HOT ELECTRON EFFECTS OF IMPORTANCE FOR MICRON AND SUBMICRON DEVICES.

FINAL REPORT

K. HESS and G. E. STILLMAN

SEPTEMBER 1981

OFFICE OF NAVAL RESEARCH

NR 322-086
N00014-79-C-0768

COORDINATED SCIENCE LABORATORY
UNIVERSITY OF ILLINOIS AT URBANA-CHAMPAIGN
URBANA, ILL. 61801

APPROVED FOR PUBLIC RELEASE;
DISTRIBUTION UNLIMITED.
During the period of this contract fifteen papers have been published. The manuscripts concern lateral transport in superlattices, transport at extremely high electric fields and impact ionization and quantum well heterojunction lasers.

1. Lateral Transport in Superlattices

A new mechanism was introduced to obtain negative differential resistance in layered heterostructures for conduction parallel to the interface. The mechanism is based on hot-electron thermionic emission from high mobility GaAs into low mobility $\text{Al}_x\text{Ga}_{1-x}\text{As}$ and represents the real space analogy to the Gunn effect (paper 1). The validity of this idea was substantiated by phenomenological treatments (paper 2), Monte Carlo Simulations (paper 3) and experiments (paper 4). This effect is vital for any high field transport application in layered structures for scaling laws of the high mobility transistor, (T. Mimura, S. Hiyamizu, T. Fujii and K. Nambu, JJAP 19, 225-227, 1980) emission of electrons into substrates, etc. Our work on this effect continues especially with respect to the possibility of fast switching and storage between layers. The interest in this effect led to the development of a fairly complete theory of transport in heterolayers which was also treated and partly expanded by B. K. Ridley and P. Price.

2. Transport at Extremely High Electric Fields and Impact Ionization

We have developed a Monte Carlo simulation of impact ionization including the bandstructure as calculated by the empirical pseudopotential method (papers 5 and 7). We chose to include bandstructure effects into transport phenomena i.e. we calculated transport at high energies while all other groups in this area rather calculate transport at high fields.
We were able to show the vital importance of the bandstructure to impact ionization phenomena and to fit our results to most existing experimental data (except for the anisotropy measured by Pearsall as pointed out in paper 6). We consider this penetration to high energies and deep into the bands as vital for the development of high field transport and continue this project to include various materials and also high scattering rates.

We also investigated impact ionization in layered structures and designed a low noise avalanche photo diode. This structure was successfully fabricated at Bell Labs (Capasso et al. IEDM to be published) and confirms our theoretical predictions (paper 8).

3. Drift at Extremely High Electric Field

A system for measuring the high field drift with the microwave time of flight technique has been set up. It is currently successfully used in a follow up project (supported by ONR).

4. Quantum Well Heterojunction Lasers

Our work on quantum well heterojunction lasers centered on theoretical aspects of the participation of hot electrons and phonons in the laser operation. The work was performed in cooperation with the group of Professor N. Holonyak, Jr. and resulted in publications on phonon contributions to laser operation (9, 10) the effect of compositional disorder on the energy of the emitted light (11), exciton recombination (12), the temperature dependence of the threshold current (13), the effect of phonon reflectors (14) and finally in a summary of the hot-electron and laser research (Physics Today paper (15)).
PREVIOUS REPORTS
The goal of this research is to understand the basic mechanisms of high-field electronic transport, drift, diffusion and generation-recombination in materials which are important or have high potential for device applications.

Progress: We have developed a computer program for high field transport which includes a realistic band structure as calculated by the empirical pseudopotential model. This numerical technique allows us to calculate impact ionization almost from first principles including the orientation dependence, energy loss by polar optical and deformation potential scattering and also spatial dependences as encountered in semiconductor heterojunctions (publications 1-3). Our investigations of transport in heterojunction layers led us to the concept of real space transfer of hot electron thermionic emission out of potential wells. This concept has, in our opinion, high potential for novel device applications (publications 1,5). Part of our research was connected with scattering processes at interfaces and with transport in quantized inversion layers. Here we assessed the importance of remote phonon scattering (publication 6). The influence of the heating of electrons to suprathermal levels on the threshold current of heterojunction lasers was investigated and it was found that the temperature dependence is reduced by these effects (publications 7,8). Finally, we investigated (in cooperation with Prof. N. Holonyak, Jr.) the influence of high phonon densities on quantum well heterojunction lasers. It was found that the phonon occupation numbers can be enhanced a factor 10 or more above the equilibrium thermodynamic average value in specific structures (publications 1-4).

Recent Publications:


Abstract for an Invited Paper

for the New York Meeting of the
American Physical Society

24-28 March 1980

Date

Real Space Transfer of Hot Electrons in Modulation-Doped Structures.*
K. HESS, University of Illinois, Urbana. (30 min.)

Electronic transport in semiconductor heterojunction layers differs from "normal" bulk transport in several respects. Electrons may be confined to a potential well (typically 0.1 - 0.5 eV deep) and therefore may be separated from their parent donors and other scattering centers which are located in neighboring layers. As a consequence of this separation, ionized impurity scattering can be strongly reduced. The scattering rate for the electron-phonon interaction is enhanced in layered structures. However, the enhancement is negligible as long as size quantization is unimportant. Other departures from bulk properties arise for hot electrons in heterojunction layers. High electric fields parallel to the interface can supply enough energy to the electrons to allow them to propagate out of the well into the confinement layers, where they experience strong scattering. A similar effect can occur in MOS-transistors, metal-semiconductor field effect transistors, and charge coupled devices as an unwelcome side effect. In modulation doped GaAs-Al$_x$Ga$_{1-x}$As heterojunction structures, however, there exists the possibility of new device applications. The transfer of electrons (in real space) from a high mobility layer (GaAs) to a low mobility layer (Al$_x$Ga$_{1-x}$As) can give rise to negative differential resistance. The similarities and differences to the Hilsum-Ridley-Watkins mechanism (k-space transfer, Gunn effect) are discussed, based on results from the method of moments and Monte Carlo calculations.4

*Supported by the Office of Naval Research and the Joint Services Electronics Program.
REAL-SPACE ELECTRON TRANSFER BY THERMIONIC EMISSION IN GaAs-Al\textsubscript{x}Ga\textsubscript{1-x}As HETEROSTRUCTURES: ANALYTICAL MODEL FOR LARGE LAYER WIDTHS†

H. SHICHIJO, K. HESS and B. G. STREETMAN

Department of Electrical Engineering and Coordinated Science Laboratory, University of Illinois at Urbana-Champaign, Urbana, IL 61801, U.S.A.

(Received 29 October 1979; in revised form 1 January 1980)

Abstract—Calculations are presented for negative differential resistance (NDR) and switching in layered GaAs-Al\textsubscript{x}Ga\textsubscript{1-x}As heterostructures with a high electric field parallel to the interface. The mechanism is based on thermionic emission of hot electrons from the GaAs layers into the Al\textsubscript{x}Ga\textsubscript{1-x}As layers. A new mechanism has been proposed to obtain negative differential resistance (NDR) in semiconductor heterostructures.[1] The basic structure of this device consists of alternating GaAs-Al\textsubscript{x}Ga\textsubscript{1-x}As multilayers, or other appropriate lattice-matched materials with dissimilar band-gap energies and carrier mobilities. It has been mentioned[1] that this mechanism may benefit from modulation doping[2, 3] of the layers. In such a structure electrons reside primarily in the Al\textsubscript{x}Ga\textsubscript{1-x}As layer, and a position-independent electron temperature and quasi-Fermi level in the narrower GaAs layer. Thermal conduction of hot electrons from the GaAs layer into the Al\textsubscript{x}Ga\textsubscript{1-x}As layer is taken into account. The results of the calculations show that the threshold electric field for the onset of NDR and the peak-to-valley ratio can be controlled to a large extent by adjusting the mobility of the Al\textsubscript{x}Ga\textsubscript{1-x}As layer, the layer dimensions, and the potential barrier (Al mole fraction in the Al\textsubscript{x}Ga\textsubscript{1-x}As).

†Supported by the Joint Services Electronics Program (U.S. Army, U.S. Navy, U.S. Air Force) under Contract Number N00014-78-C-0424, and the Office of Naval Research under Contract Number N00014-76-C-0768.

NOTATION

\(E_0\) effective field strength \(E_0 = \text{mean} \left( \frac{1}{e} - \frac{1}{e_0} \right)/4\pi\epsilon\)

\(E_{\text{QF}}\) Quasi-Fermi level in the GaAs layer

\(E_{\text{QF}}\) position-dependent Quasi-Fermi level in the Al\textsubscript{x}Ga\textsubscript{1-x}As layer by

\(e\) energy of the electron

\(F\) applied electric field

\(h_{\text{opt}}\) optical phonon energy in the GaAs

\(h_{\text{QF}}\) thermionic current from the GaAs layer to the Al\textsubscript{x}Ga\textsubscript{1-x}As layer

\(h_{\text{QF}}\) thermionic current from the Al\textsubscript{x}Ga\textsubscript{1-x}As layer to the GaAs layer

\(K_0\) Bessel function of order 0

\(K_1\) Bessel function of order 1

\(e\), \(k\) components of the electron wave vector

\(L_x\) width of the GaAs layer

\(L_x\) width of the Al\textsubscript{x}Ga\textsubscript{1-x}As layer

\(m_e\) electron effective mass in GaAs

\(m_{\text{QF}}\) electron effective mass in Al\textsubscript{x}Ga\textsubscript{1-x}As

\(N\) total number of electrons in the system

\(N_e\) number of electrons in the GaAs layer

\(N_x\) number of electrons in the Al\textsubscript{x}Ga\textsubscript{1-x}As layer

\(T_0\) lattice temperature

\(T_e\) electron temperature in the GaAs

\(T_{\text{QF}}\) position-dependent electron temperature in the Al\textsubscript{x}Ga\textsubscript{1-x}As layer

\(\Delta E\) potential barrier height

\(\mu_e\) electron mobility in GaAs

\(\mu_x\) electron mobility in Al\textsubscript{x}Ga\textsubscript{1-x}As

1. INTRODUCTION

Negative differential effects, typified by the tunnel diode and the Gunn diode, are of fundamental interest and are also important for their possible applications to microwave, switching, and memory devices. Recently a new mechanism has been proposed to obtain negative differential resistance (NDR) in semiconductor heterostructures[1]. The basic structure of this device consists of alternating GaAs-Al\textsubscript{x}Ga\textsubscript{1-x}As multilayers, or other appropriate lattice-matched materials with dissimilar band-gap energies and carrier mobilities. It has been mentioned[1] that this mechanism may benefit from modulation doping[2, 3] of the layers. In such a structure electrons reside primarily in the Al\textsubscript{x}Ga\textsubscript{1-x}As layer, and a position-independent electron temperature and quasi-Fermi level in the narrower GaAs layer. Thermal conduction of hot electrons from the GaAs layer into the Al\textsubscript{x}Ga\textsubscript{1-x}As layer is taken into account. The results of the calculations show that the threshold electric field for the onset of NDR and the peak-to-valley ratio can be controlled to a large extent by adjusting the mobility of the Al\textsubscript{x}Ga\textsubscript{1-x}As layer, the layer dimensions, and the potential barrier (Al mole fraction in the Al\textsubscript{x}Ga\textsubscript{1-x}As).
dependent electron temperature and Fermi level in the AlGaAs layer. Special attention is given to the degree of control of the device characteristics by the adjustment of the following parameters: the mobility of the AlGaAs layer; the layer dimensions; the Al mole fraction; and therefore the potential barrier height.

2. ANALYTICAL CONSIDERATIONS

Figure 1 shows schematically the band structure, doping distribution, and electron mobility of modulation-doped GaAs-AlGaAs layers. The AlGaAs layers are intentionally doped to a density of \(10^{17} \sim 10^{18}\) cm\(^{-3}\), whereas the GaAs layers contain only unintentional background impurities \(10^{14} \sim 10^{15}\) cm\(^{-3}\). At thermal equilibrium, the electrons reside at the minimum of the potential wells, i.e. in the GaAs layers. When separated from their parent donors by more than 200 Å these electrons experience strongly reduced impurity scattering [2, 4]. Therefore, for a typical layer thickness of 400 Å, the electron mobility in the GaAs layer will be very high \((\approx 5000\) cm/V sec at 300 K\). Dingle et al. have experimentally observed a mobility of 5000 cm/V sec at 300 K, and even higher mobilities \((\sim 15000\) cm/V sec\) at lower temperatures [2]. The AlGaAs layers can be made strongly compensated, and thereby the mobility in these layers can be very low \((\sim 500\) cm/V sec or less\). Application of a high electric field parallel to the layer interfaces of this structure will result in heating of the high mobility electrons in the GaAs layer only. When the mean kinetic energy of these electrons becomes comparable to the potential barrier height, they can be thermionically emitted into the AlGaAs layer. During the transfer from the high mobility GaAs layer to the low mobility AlGaAs layer, the sample should exhibit negative differential resistance.

The problem is complicated by the fact that some of the cooler electrons in the AlGaAs can undergo reverse transfer into the GaAs layer. In order to take account of this energy and momentum exchange between the GaAs and the AlGaAs layers, one must solve the Boltzmann equation:

\[
\frac{d\rho}{d\tau} + \frac{1}{\hbar} \mathbf{F} \cdot \nabla \rho - v \cdot \nabla \rho = \frac{d\rho}{dt},
\]

with appropriate boundary conditions. Due to the complexity of the boundary conditions in the case of real space transfer, an explicit expression for the distribution function cannot be obtained. Therefore we assume a Maxwellian form for the isotropic part of the distribution function, with a position-dependent electron temperature. This assumption is justified by the fact that the electron density is high in the GaAs layer at the start of the electron transfer, since the AlGaAs layer collects electrons from the neighboring layers. Typically the GaAs layer will have an electron density of \(10^{18} \sim 10^{19}\) cm\(^{-3}\). Electron-electron collisions will therefore randomize the energy gained in the electric field direction and establish a Maxwellian distribution. Above the band edge of the AlGaAs, the electrons in the GaAs will follow the coordinate system used for the calculations.

The coordinate system is in the y-direction and represents the drift electric field as usual. The third term is the Fermi level term, the rate of change of the Fermi level in the GaAs due to the thermal equilibrium conditions at the Fermi level. This term on the right represents the Fermi level change due to the statistical distribution of the impurities.

For a typical layer thickness of 400 Å, this term is in the order of magnitude of the Fermi energy. The second term on the right represents the contribution from size quantization effects and other contributions arising from modulation-doped layers. The method of obtaining the equations of motion is to use the semiclassical Boltzmann equation. With large layer widths, the potential fluctuations due to the statistical distribution of the impurities can also be neglected. Suppose that the transfer speed is slower for large layers, which is not considered here.

Figure 2 shows the model used in the calculations. We assume a position-dependent electron temperature, \(T_i(x)\), and Fermi level, \(E_F(x)\), in the AlGaAs layer. Because of the small dimensions, the use of the quasi-Fermi level is justified only at very high electron densities. Similar methods have recently been employed by others [5] to analyze the thermionic emission in metal-semiconductor contacts. In the independent electron model, \(E_F\), with this assumption of Fermi level in the AlGaAs layer, the distribution of hot electrons is defined as \(T_i(x)\) at the interface of the AlGaAs layer.

where \(T_i(x)\) is the Maxwellian form at position \(x\) and \(E_F(x)\) is the Fermi level at position \(x\). The coordinate system is in the y-direction, which represents the drift electric field as usual. The third term is the Fermi level term, the rate of change of the Fermi level in the GaAs due to the thermal equilibrium conditions at the Fermi level. This term on the right represents the Fermi level change due to the statistical distribution of the impurities.

For a typical layer thickness, this term is in the order of magnitude of the Fermi energy. The second term on the right represents the contribution from size quantization effects and other contributions arising from modulation-doped layers. The method of obtaining the equations of motion is to use the semiclassical Boltzmann equation. With large layer widths, the potential fluctuations due to the statistical distribution of the impurities can also be neglected. Suppose that the transfer speed is slower for large layers, which is not considered here.

Figure 2 shows the model used in the calculations. We assume a position-dependent electron temperature, \(T_i(x)\), and Fermi level, \(E_F(x)\), in the AlGaAs layer. Because of the small dimensions, the use of the quasi-Fermi level is justified only at very high electron densities. Similar methods have recently been employed by others [5] to analyze the thermionic emission in metal-semiconductor contacts. In the independent electron model, \(E_F\), with this assumption of Fermi level in the AlGaAs layer, the distribution of hot electrons is defined as \(T_i(x)\) at the interface of the AlGaAs layer.

where \(T_i(x)\) is the Maxwellian form at position \(x\) and \(E_F(x)\) is the Fermi level at position \(x\). The coordinate system is in the y-direction, which represents the drift electric field as usual. The third term is the Fermi level term, the rate of change of the Fermi level in the GaAs due to the thermal equilibrium conditions at the Fermi level. This term on the right represents the Fermi level change due to the statistical distribution of the impurities.

For a typical layer thickness, this term is in the order of magnitude of the Fermi energy. The second term on the right represents the contribution from size quantization effects and other contributions arising from modulation-doped layers. The method of obtaining the equations of motion is to use the semiclassical Boltzmann equation. With large layer widths, the potential fluctuations due to the statistical distribution of the impurities can also be neglected. Suppose that the transfer speed is slower for large layers, which is not considered here.

Figure 2 shows the model used in the calculations. We assume a position-dependent electron temperature, \(T_i(x)\), and Fermi level, \(E_F(x)\), in the AlGaAs layer. Because of the small dimensions, the use of the quasi-Fermi level is justified only at very high electron densities. Similar methods have recently been employed by others [5] to analyze the thermionic emission in metal-semiconductor contacts. In the independent electron model, \(E_F\), with this assumption of Fermi level in the AlGaAs layer, the distribution of hot electrons is defined as \(T_i(x)\) at the interface of the AlGaAs layer.
GaAs contacts. In the GaAs layer we assume a position-independent electron temperature, $T_e$, and Fermi level, $E_F$. With this assumption we only need to solve for the position dependence of the electron temperature and the Fermi level in the Al$_{x}$Ga$_{1-x}$As layers. The thermal conduction of hot electrons from the GaAs layer into the Al$_{x}$Ga$_{1-x}$As layers is then accounted for by the slope of $T_e(x)$ at the interface boundary. Although at the boundary the slope of $T_e$ in the GaAs layer is zero, we assume that the same amount of energy (as given by the Fermi level) is transferred perpendicular to the electric field. This term is given after Bethel by:

\[ \mu_e F = \frac{\mu_e F L}{2e} \frac{dE_F}{dx} - \frac{dE_F}{dx} \rho_{\text{osc}} \]

where $Z = \frac{kT_e}{\hbar v_F}$ and $\mu$ is the mobility in the GaAs. When only polar optical scattering is operative, this mobility is given by:

\[ \mu_e = \frac{3\sqrt{\pi} \left( \frac{2\hbar v_F}{eT_e} \right)^{1/2}}{2 \pi k^2 \hbar^2 N_x} \left( \frac{Z}{Z_o} \right)^{1/2} \exp \left( - \frac{Z}{Z_o} \right) \left[ \exp \left( Z - Z_o \right) - 1 \right] K_i(z/2) + \left[ \exp \left( Z - Z_o \right) - 1 \right] K_0(z/2). \]

The second term on the right side of eqn. (6) represents the power flowing out of the GaAs into the Al$_{x}$Ga$_{1-x}$As layers. $T_e(x)$ and $dE_F(x)$ are evaluated at the boundary $x = 0$. We have used the fact that this power flow is due only to those electrons in the GaAs with energy higher than the Al$_{x}$Ga$_{1-x}$As band edge. Equations (4) combined with eqn (5) is now solved numerically with the boundary condition $T_e(0) = T_e$.

To determine the quasi-Fermi levels, $E_{F1}$ and $E_{F2}$, we need two additional conditions. One is obtained from the condition $j_e = 0$. We simplify this condition to the balance of the thermionic currents in both directions at the interface. Under collision-free transport conditions the thermionic current $j_{e1}$, from the GaAs to the Al$_{x}$Ga$_{1-x}$As, is given after Bethel by:

\[ j_{e1} = \frac{c^2 m^*}{2 \pi k^3 T_e} \left( \frac{K_1(z)}{K_0(z)} \right) \exp \left( \frac{E_{F1} - \Delta E}{kT_e} \right) \]

\[ j_{e2} = \frac{c^2 m^*}{2 \pi k^3 T_e} \left( \frac{K_1(z)}{K_0(z)} \right) \exp \left( \frac{E_{F2} - \Delta E}{kT_e} \right). \]

The current $j_{e1}$ flowing from the Al$_{x}$Ga$_{1-x}$As to the GaAs layer is:

\[ j_{e1} = \frac{c^2 m^*}{2 \pi k^3 T_e} \left( \frac{K_1(z)}{K_0(z)} \right) \exp \left( \frac{E_{F1} - \Delta E}{kT_e} \right). \]

where $T_e$ is evaluated at $x = 0$. Under steady-state conditions we have $j_{e1} = j_{e2}$. The other additional condition arises from conservation of the total number of electrons, $N = N_1 + N_2$. $N_1$ and $N_2$ are calculated using the electron temperature and Fermi level in each layer.

The set of layer equations obtained is given below:

\[ \frac{(2\hbar v_F)}{m^*} \frac{d^2}{dx^2} \left[ \left( \frac{dE_F}{dx} \right) \exp \left( \frac{E_{F1} - \Delta E}{kT_e} \right) \right] \frac{d^2}{dx^2} \left[ \left( \frac{dE_F}{dx} \right) \exp \left( \frac{E_{F2} - \Delta E}{kT_e} \right) \right] \]

where $Z_e = \frac{kT_e}{\hbar v_F}$ and $Z_o = \frac{kT_o}{\hbar v_F}$, and the position dependences of $E_F(x)$ and $T_e(x)$ have been omitted. The left side of eqn (4) is the rate of energy loss due to polar optical scattering[6], and the first term on the right side is the power input from the applied electric field. The second term on the right represents the energy flow from the GaAs due to the transfer of hot electrons. With the assumption of energy conservation at the boundary, we can then obtain a similar power balance equation relating $T_e$ and $F$ (electric field) in the GaAs layer:

\[ \frac{(2\hbar v_F)}{m^*} \frac{d^2}{dx^2} \left[ \left( \frac{dE_F}{dx} \right) \exp \left( \frac{E_{F1} - \Delta E}{kT_e} \right) \right] \frac{d^2}{dx^2} \left[ \left( \frac{dE_F}{dx} \right) \exp \left( \frac{E_{F2} - \Delta E}{kT_e} \right) \right] \]

\[ \frac{(2\hbar v_F)}{m^*} \frac{d^2}{dx^2} \left[ \left( \frac{dE_F}{dx} \right) \exp \left( \frac{E_{F1} - \Delta E}{kT_e} \right) \right] \frac{d^2}{dx^2} \left[ \left( \frac{dE_F}{dx} \right) \exp \left( \frac{E_{F2} - \Delta E}{kT_e} \right) \right] \]

\[ \mu_e = \frac{3\sqrt{\pi} \left( \frac{2\hbar v_F}{eT_e} \right)^{1/2}}{2 \pi k^2 \hbar^2 N_x} \left( \frac{Z}{Z_o} \right)^{1/2} \exp \left( - \frac{Z}{Z_o} \right) \left[ \exp \left( Z - Z_o \right) - 1 \right] K_i(z/2) + \left[ \exp \left( Z - Z_o \right) - 1 \right] K_0(z/2). \]
The position of the GaAs potential well is shown in the dashed line. The variation of the fraction of electrons in the GaAs layer for various mobilities in the AlGaAs layer characteristics is and hence the transfer of electrons into the AlGaAs layer. For purposes of comparison we include in Fig. 6 (insert) the velocity-field characteristics calculated by Fawcett et al. in 1970 for the Gunn effect[13]. The parameter for their curves was the inter-valley deformation potential.

The two sets of curves in Fig. 6 show surprisingly similar features. Actually, our discussion of real space transfer almost parallels that of the Gunn effect, but with two crucial differences. First, in our mechanism electrons leave the high mobility GaAs layer by thermionic emission and are transferred in real space to the low-mobility AlGaAs layer; on the other hand, electrons in the Gunn effect leave the high mobility GaAs layer by tunneling and are transferred in real space to the low-mobility AlGaAs layer.

The transfer is larger for smaller mobility values, a consequence of the greater carrier heating for smaller mobility as seen in Fig. 3. Here again the analogy with the Gunn effect should be noted[12].

The current-voltage characteristics are straightforward to calculate from this model. The results of the calculations are shown in Fig. 6. The magnitude of the NDR changes dramatically with the mobility in the AlGaAs layer. For purposes of comparison we include in Fig. 6 (insert) the velocity-field characteristics calculated by Fawcett et al. in 1970 for the Gunn effect[13]. The parameter for their curves was the inter-valley deformation potential.

The two sets of curves in Fig. 6 show surprisingly similar features. Actually, our discussion of real space transfer almost parallels that of the Gunn effect, but with two crucial differences. First, in our mechanism electrons leave the high mobility GaAs layer by thermionic emission and are transferred in real space to the low-

mobile AlGaAs layer; on the other hand, electrons in the Gunn effect leave the high mobility GaAs layer by tunneling and are transferred in real space to the low-mobility AlGaAs layer.

The transfer is larger for smaller mobility values, a consequence of the greater carrier heating for smaller mobility as seen in Fig. 3. Here again the analogy with the Gunn effect should be noted[12].

The current-voltage characteristics are straightforward to calculate from this model. The results of the calculations are shown in Fig. 6. The magnitude of the NDR changes dramatically with the mobility in the AlGaAs layer. For purposes of comparison we include in Fig. 6 (insert) the velocity-field characteristics calculated by Fawcett et al. in 1970 for the Gunn effect[13]. The parameter for their curves was the inter-valley deformation potential.

The two sets of curves in Fig. 6 show surprisingly similar features. Actually, our discussion of real space transfer almost parallels that of the Gunn effect, but with two crucial differences. First, in our mechanism electrons leave the high mobility GaAs layer by thermionic emission and are transferred in real space to the low-

mobile AlGaAs layer; on the other hand, electrons in the Gunn effect leave the high mobility GaAs layer by tunneling and are transferred in real space to the low-mobility AlGaAs layer.

The transfer is larger for smaller mobility values, a consequence of the greater carrier heating for smaller mobility as seen in Fig. 3. Here again the analogy with the Gunn effect should be noted[12].

The current-voltage characteristics are straightforward to calculate from this model. The results of the calculations are shown in Fig. 6. The magnitude of the NDR changes dramatically with the mobility in the AlGaAs layer. For purposes of comparison we include in Fig. 6 (insert) the velocity-field characteristics calculated by Fawcett et al. in 1970 for the Gunn effect[13]. The parameter for their curves was the inter-valley deformation potential.

The two sets of curves in Fig. 6 show surprisingly similar features. Actually, our discussion of real space transfer almost parallels that of the Gunn effect, but with two crucial differences. First, in our mechanism electrons leave the high mobility GaAs layer by thermionic emission and are transferred in real space to the low-

mobile AlGaAs layer; on the other hand, electrons in the Gunn effect leave the high mobility GaAs layer by tunneling and are transferred in real space to the low-mobility AlGaAs layer.
mobility Al,Ga_,As layer in real space to the low-

energy Al,Ga_,As layer. In the Gunn effect, on the
other hand, electrons transfer from one valley of high
mobility to another of low mobility or high-space. A second, and most important distinction is the
fact that our device characteristics can be controlled to a
higher degree than with a device utilizing the Gunn
effect. As already seen in Fig. 6 (insert), the curves for
the Gunn effect have as a parameter the intervalley de-
formation potential, which is a material property and cannot
be changed. On the other hand, the parameter in Fig. 6
for the real-space transfer process is the mobility of the
Al,Ga',As layer, which can be controlled by adjusting
the doping of the layer. The characteristics can also be
changed by varying other device parameters, such as the
layer dimensions and the potential barrier height. For
example, the potential barrier height can be controlled by
to changing the Al mole fraction of the Al,Ga',As. The
effect of varying this parameter on the current-voltage
characteristics is shown in Fig. 7. For this particular set
of parameters the threshold field for the onset of NDR
can be varied between 2 and 3 kV/cm and the peak-to-
valley ratio between 1.3 and 2.0. We have also examined
the effects of the operating temperature and as expected,
the NDR is more pronounced at lower temperatures.

Finally, we would like to summarize the simplification
of our model. As shown in Fig. 2, we have ignored the
band-bending caused by the ionized donors. This effect
can be quite large for heavily doped Al,Ga',As layers.
The ionized donors create an electric field at the GaAs-
Al,Ga',As interface which tends to pull the hot elec-
trons toward the Al,Ga',As layer. Therefore, we be-
lieve that the band-bending due to ionized donors should
aid the transfer of electrons into the low-mobility
Al,Ga',As layers. Of course, as greater numbers of
electrons are transferred, the effect becomes smaller
since more ionized donors are neutralized. This band-
bending effect is also reduced for compensated
Al,Ga',As layers. Secondly, we have not taken into
account the effects of the conduction band L minima,
which are known to be located approximately 330 meV
above the Γ minimum of GaAs. We have deliberately
chosen values of ΔE such that these L minima are above
the band edge of the Al,Ga',As [see for example, Fig.

7]. As the Al,Ga',As band edge approaches the GaAs
L minima, some electrons may be transferred to these L
minima by intervalley scattering before they undergo
transfer in real space to the AL,Ga',As layer. However,
Monte Carlo calculations[14] show that the effects of the
L minima are negligible and that real space transfer
dominates over intervalley scattering even for a barrier
height of ΔE = 200 meV. For values of ΔE = 350 meV
and more, however, the effect of the L minima can be
considerable. In fact, by intentionally aligning the
Al,Ga',As band edge to the energy value of the L
minima in GaAs, the Gunn effect can be enhanced by
real space transfer, and larger peak-to-valley ratios
should result. Third and finally, we have neglected the
quantum mechanical reflection of electrons at the GaAs-
Al,Ga',As interface. Wu and Yang[15] have obtained
the formula for the three-dimensional transmission
coefficient at a heterostructure interface using quantum
mechanical considerations. When an electron with an
energy of 230 meV is moving perpendicular to an inter-
face with a barrier height of 200 meV, we obtain a
transmission coefficient value of 75% using their formula.
Therefore, some electrons are reflected into the GaAs
layer when trying to cross the interface. Similarly, some
of those electrons which have already transferred into
the Al,Ga',As are also reflected at the interface.

The effects of thermionic emission can also be used to
construct a high-speed switch. If the GaAs and the
Al,Ga',As layers are contacted separately, voltages
can be applied independently to the two materials or
between them. There will be a negligible current in the
Al,Ga',As until an appreciable fraction of electrons are
emitted from the GaAs. Figure 8 illustrates this switching
effect. The electric field to the Al,Ga',As is kept con-
stant at 12 kV/cm. The GaAs and the Al,Ga',As cur-
rents can be switched on and off by the electric field
applied to the GaAs layer. The dotted curve is obtained
in the case of no thermal conduction. Since the transfer
times in this mechanism are short (~10-11 sec), a
high-speed switch can be envisioned. Extensions of the
real space transfer mechanism might include variation of
the effective barrier height by application of voltage
between the layers, detection of optical excitations from the GaAs well by monitoring the Al$_x$Ga$_{1-x}$As conductivity, and other applications.

4. CONCLUSIONS

We have described a mechanism to obtain negative differential resistance and switching in layered GaAs-Al$_x$Ga$_{1-x}$As heterostructures with high electric fields applied parallel to the interfaces. The mechanism is based on thermionic emission of hot electrons from high mobility GaAs layers into low mobility Al$_x$Ga$_{1-x}$As layers. An analytical model has been presented in the limit of large layer width, typically 400 Å or wider. We have employed the method of moments to solve the Boltzmann equation assuming a position-dependent electron temperature, $T_e(x)$, and Fermi level, $E_F(x)$, in the Al$_x$Ga$_{1-x}$As layer and a position-independent electron temperature, $T_e$, and Fermi level, $E_F$, in the GaAs layer. The thermal conduction of hot electrons from the GaAs layers into the Al$_x$Ga$_{1-x}$As layers is taken into account. As a consequence, the power balance equation contains an additional term. The resulting differential equation for $T_e(x)$ has been solved numerically. The results of the calculations show the device characteristics are similar to those for the Gunn effect. The crucial difference between the Gunn effect and the real-space transfer mechanism is that our device characteristics can be engineered by adjusting various parameters. The effects of changing the mobility in the Al$_x$Ga$_{1-x}$As layers are apparent from Figs. 5 and 6. The characteristics can also be varied by changing the layer dimensions and Al mole fraction (potential barrier height, Fig. 7). This degree of control of device characteristics makes the real-space transfer mechanism especially attractive for various applications.

Acknowledgements—We would like to thank Prof. H. Morkoc and J. Oberstar for helpful discussions.

REFERENCES


11. See Fig. 16 of Ref. [10].

12. See Fig. 14 of Ref. [10].


Monte Carlo simulation of real-space electron transfer in GaAs-AlGaAs heterostructures

T. H. Glisson, J. R. Hauser, and M. A. Littlejohn
Department of Electrical Engineering, North Carolina State University, Raleigh, North Carolina 27650
K. Hess, B. G. Streetman, and H. Shichijo
Department of Electrical Engineering and Coordinated Science Laboratory, University of Illinois at Urbana-Champaign

(Received 13 March 1980; accepted for publication 11 June 1980)

The Monte Carlo method has been used to simulate electron transport in GaAs/AlGaAs heterostructures with an electric field applied parallel to the heterojunction interface. The simulations indicate that a unique physical mechanism for negative differential conductivity is provided by such layered heterostructures, which is analogous in many respects to the Gunn effect. This mechanism has been termed "real-space electron transfer" since it involves the transfer of electrons from a high-mobility GaAs region to an adjacent low-mobility AlGaAs region as the applied electric field intensity is increased. The simulations further indicate that the important details of the resulting velocity-field characteristics for these layered heterostructures can be controlled primarily through material doping densities, layer thicknesses, and the material properties of the individual layers. Thus, the phenomenon of real-space electron transfer potentially provides the ability to "engineer" those basic material properties which influence the performance of negative resistance devices.

PACS numbers: 72.20.Jv, 72.80.Ey

I. INTRODUCTION

In a recent paper a new mechanism for obtaining negative differential conductivity in layered heterostructures was described. This mechanism is based on the transfer of hot electrons from high-mobility GaAs layers sandwiched between adjacent low-mobility Al, Ga$_1$$_x$ As layers. The resulting negative differential conductivity is analogous to the Gunn effect, except that the electrons are transferred in real space rather than in momentum space.

To properly describe real-space electron transfer, it is necessary to account for the scattering mechanisms encountered by electrons being transported at high kinetic energies in the potential well in the GaAs, which exists due to the conduction band discontinuity between GaAs and AlGaAs. A mechanical analogy to real-space transfer is provided by the example of a ball rolling down a chute. The ball will stay in the chute if its kinetic energy remains small. However, if the ball gains adequate kinetic energy, then an obstacle can scatter the ball out of the chute. A similar effect occurs in a layered heterostructure where electrons drift in the potential well under the influence of a high electric field. If the mobilities inside and outside the well can be controlled, then the transfer of electrons from the well can be used to control the current-voltage characteristics of the heterostructure device. If the mobility outside the well is much lower than that inside, the effect results in a negative differential conductivity.

In the previous paper, the real-space transfer effect was examined on the basis of "thermionic emission currents"; that is, the densities of electrons inside and outside the well were calculated by balancing the Richardson currents. In these calculations the layers were treated independently, and energy exchange between the layers was not considered. The energy distribution of the electrons in both layers was assumed to be Maxwellian, with the GaAs at an elevated temperature $T_A$ and with the temperature in the Al, Ga$_1$$_x$ As assumed to be equal to the lattice temperature $T_L$. This model has four essential deficiencies: (i) It is well known that at high electric fields the energy distribution functions in polar semiconductors are highly non-Maxwellian. (ii) There is an energy exchange between the layers because energetic carriers are flowing out of the GaAs and cold carriers are returning. (iii) The model does not account for electron temperature gradients or electron-electron interactions. (iv) The complicated band structure of the multilayer heterojunctions (e.g., the role of the $L$ minima in the two materials) was not considered.

It is possible to include (ii) and (iii) in a simple theory using the method of moments. This type of calculation is described elsewhere. The only calculation capable of simultaneously including (i), (ii), and (iv), however, is a Monte Carlo calculation. The purpose of this paper is to describe the results of a Monte Carlo study of real-space transfer in GaAs/AlGaAs layered heterostructures. The Monte Carlo calculations predict a negative differential conductivity for properly chosen heterostructures. The advantage of this negative resistance mechanism over the normal Gunn effect is that all the essential materials parameters can be "engineered". For example, the peak-to-valley ratio can be controlled by the layer width and mobility ratio (including modulation doping), the onset of the negative differential resistance can be controlled by the Al mole fraction (barrier height), and finally the speed of the device can be controlled by the layer thicknesses. We also show that the real-space transfer effect should occur well before the Gunn effect (k-space transfer) for junction barrier heights of approximately 200 meV in GaAs/Al, Ga$_1$$_x$ As heterostructures.
II. THE TRANSPORT MODEL

The model used in the calculations is classical in the sense that the transport equations are based on the quasiclassical approximation normally employed in the Monte Carlo method. The essential features of the simulation procedures have been presented previously. These procedures were modified for the present work in order to allow the Monte Carlo method to be applied to the material/device configuration shown schematically in Fig. 1. The model assumes an abrupt potential barrier of height $\Delta E$ in the GaAs, and band bending effects are neglected. The electric field created by the ionized donors in the space-charge region of the heterojunction is also neglected. This field tends to attract energetic electrons from the GaAs into the Al,Ga, As. Hence it would enhance the transfer out of the well and impede transfer back into the well. This would enhance the negative resistance effect reported here. The importance of the exact nature of the potential barrier will be difficult to ascertain. An exact treatment should of course include a self-consistent calculation of the potential barrier. In practice, however, the ideal potential barrier can be closely approximated by suitable doping profiles and compensation in the AlGaAs.

The well layer thickness $d_1$ is assumed to be large enough for size quantization effects to be negligible. For layer thicknesses greater than 400 Å size quantization effects are not important at room temperature. Therefore, these effects are even less important for the hot-electron problem investigated in this work.

Bulk material parameters are used in the simulation of the transport in the two regions of the heterostructure. The parameters for the GaAs have been reported previously. The use has resulted in values for both low-field mobility and hot-electron velocity-field characteristics which are in good agreement with experiment. The material parameters for the Al,Ga, As are determined from either measured experimental values or by the use of an interpolation procedure. These parameters depend on the alloy composition $x$. The value of $x$ is obtained from the desired barrier height $\Delta E$, the known energy-band structure of AlGaAs, and the accepted conduction-band alignment scheme of the GaAs/AlGaAs system. The electrons drift in a uniform electric field applied in the $y$ direction parallel to the heterojunction interface. The one-electron simulation begins by releasing an electron from the center of the GaAs well with thermal ($T = 300$ K) energy and in a randomly selected direction. The electron then undergoes scattering interactions in the normal Monte Carlo framework. The scattering mechanisms considered in these calculations include acoustic-phonon scattering, optical-phonon scattering, piezoelectric scattering, equivalent and nonequivalent intervalley scattering, ionized impurity scattering, and random potential alloy scattering in the Al,Ga, As. In the calculations reported here only the $f(000)$ and $L(\bar{1}11)$ conduction bands are considered for GaAs, and only the $f(000)$ conduction band is considered in Al,Ga, As. This represents adequate band structure details to illustrate the essential features of real-space transfer in GaAs/AlGaAs heterostructures.

The basic heterostructure cell as shown in Fig. 1 is cyclically repeated in the Monte Carlo simulation. This is accomplished in the following manner. An electron which has the correct energetics to transfer from GaAs to AlGaAs across the boundary at $x = 0$ in Fig. 1 is made to enter the AlGaAs at $x = d_1 + d_2$ with the same energetics. Likewise, an electron that transfers from the AlGaAs to GaAs at $x = d_1 + d_2$ is made to enter the GaAs at $x = 0$ with the same energetics. The average drift velocities in the individual materials and the average velocity in the heterostructure are calculated using standard velocity estimators. Since the drift velocity in the AlGaAs is often very low ($\sim 10^4 - 10^6$ cm/sec), the total number of interactions used in the simulation must often be very large ($\sim 250,000$) in order to obtain accurate velocity estimates.

The transmission of the electrons across the boundary has been modeled in two ways. First, a classical transmission model based on conservation of energy and momentum was used. This requires a particle with inadequate energy to be ideally reflected with no energy loss, with reversal of its momentum perpendicular to the barrier and no change in momentum parallel to the barrier. Second, the quantum-mechanical transmission coefficient described by Wu and Yang was used in the simulation. Within the statistical error of the simulation no substantial differences in the results have been observed between these two transmission models.
Carrier compensation is utilized in order to vary the mobility of electrons in the AlGaAs. The free-electron density in the scattering rate for ionized impurity scattering is taken to be $10^{17}$ cm$^{-3}$, while the net ionized impurity density is allowed to vary from $10^{17}$ cm$^{-3}$ to $10^{20}$ cm$^{-3}$. This varies the electron mobility in the AlGaAs from about 4000 to 50 cm$^2$/V sec. The low-field mobility in the GaAs is held constant at about 8000 cm$^2$/V sec by taking the ionized impurity density in the GaAs to be zero.

### III. SIMULATION RESULTS

The model and procedures described in Sec.II were used to simulate the electron transport in GaAs/AlGaAs heterostructures with various device thicknesses, barrier heights, and other AlGaAs material parameters. Figure 2 shows the steady-state drift velocity of such a structure for the case where the low-field mobility of GaAs is 8000 cm$^2$/V sec and that in AlGaAs is about 500 cm$^2$/V sec. Here, the ionized impurity density in AlGaAs is $10^{19}$ cm$^{-3}$ and the barrier height is 0.2 eV. In this figure the drift velocity in the device structure is compared to that for GaAs and AlGaAs. The transport in AlGaAs remains essentially ohmic for the range of electric fields shown in Fig. 2, although at fields of near 15 kV/cm the transport in the AlGaAs would become nonlinear and would eventually exhibit velocity saturation. The peak velocity for the real-space transfer structure is $1.6 \times 10^7$ cm/sec and the threshold field is about 2.4 kV/cm. The onset of electron transfer to the AlGaAs occurs at a field of about 2 kV/cm, as can be seen in Fig. 3. This figure, which shows the relative numbers of electrons in the two adjacent materials, illustrates that for the material thicknesses and barrier height used a substantial number of electrons remain in the GaAs, even for fields well above threshold. The ratio of electrons in the two materials largely determines the peak-to-valley ratio of the real-space transfer device. This is illustrated in Fig. 4 which shows the velocity-field characteristics for the same material parameters as in Fig. 2 except that the AlGaAs mobility is reduced to about 50 cm$^2$/V sec. Here the peak velocity is essentially the same as before, although the peak-to-valley velocity ratio has been increased by a factor of 2 (valley taken at 8 kV/cm). In this case, at 8 kV/cm fewer than 10% of the electrons remain in the GaAs. The peak velocity of $1.6 \times 10^7$ cm/sec, threshold field of 2.8 kV/cm, peak-to-valley ratio of 4, and a negative mobility magnitude above threshold of greater than $10^7$ cm$^2$/V sec in this case are very attractive parameters for Gunn-type device considerations. Figures 2 and 4 support the general features of real-space electron transfer described.
by Hess et al. based on thermionic currents and the method of moments.1,4

Figure 5 shows a velocity-field characteristic when the AlGaAs mobility is 4000 cm²/V sec. Here, a substantial number of electrons remain in the GaAs for fields well above 8 kV/cm, and the two materials are equally important in determining the drift velocity in the heterostructure for fields above the threshold field of GaAs. This figure serves to illustrate that a layered heterostructure device might be used to achieve an adjustable velocity-saturation mechanism with very small or negligible negative resistance where the saturation velocity is well above the value normally obtained in silicon or indirect band gap AlGaAs ternary systems. It is worth noting that in Fig. 5 there is a slight negative differential conductivity in the AlGaAs even though only the central valley was used in the simulation. This is due to the nonparabolic nature of the central conduction band; the details of this effect have been discussed previously.4

Since the threshold field in the heterostructure device is near that for GaAs, an attempt was made to assess the importance of intervalley scattering in the GaAs and AlGaAs on the velocity-field characteristic of the structure. The satellite L(III) valley in GaAs was removed from the simulation model, and the velocity-field characteristics were calculated for barrier heights up to 0.3 eV, which is near the $\Gamma$-L intervalley separation for GaAs proposed by Aspnes.5,12 Within the statistical accuracy of the velocity estimator $n^*$ differences could be observed in the results compared to those given in Fig. 2. In addition, Fig. 6 shows the average energy of the electrons in the AlGaAs as a function of electric field for a barrier height of 0.3 eV compared to the $\Gamma$-L energy separation in the AlGaAs. For this case between 2 and 4 kV/cm the average energy is well below the intervalley energy separation, although the electrons are becoming hot. At higher electric field ($\sim$ 8 kV/cm) intervalley scattering in the AlGaAs will be important and will probably affect the peak-to-valley ratio, although it appears to influence neither the threshold field nor the peak velocity. Further studies are underway to examine the importance of scattering in the $L$ and $X$ valleys of AlGaAs.

Further aspects of the phenomenon of real-space transfer are shown in Fig. 7. This figure illustrates the influence on the heterostructure velocity-field characteristics of varying the barrier height while maintaining fixed material thicknesses. Obviously, as the barrier height increases, the velocity-field characteristic approaches that for lightly doped GaAs. This is the expected behavior, although one might expect some additional influence if the layers are thin enough for size quantization effects to be important. In addition, the form of scattering at the GaAs/AlGaAs interface could effect the electron transport in the GaAs well material. In this paper specular interface scattering has been used.

Thus, the energy and momentum relaxation mechanisms in the well material are the same as those an electron would encounter in bulk GaAs. Future studies of real-space transfer will include size quantization effects and other physical forms of interface scattering.

As the barrier height decreases in the real-space transfer simulation model, the velocity-field characteristic is increasingly influenced by the heavily compensated Al$_{1-x}$Ga$_x$As. Physically, for the material systems used here, as the barrier height decreases $x$ approaches unity. Thus, the device would consist of alternating layers of thin, lightly doped GaAs and thicker, heavily compensated

![Figure 7: Velocity-field characteristic for real-space transfer device with barrier height as a parameter. All other parameters are the same as in Fig. 2.](Image)

![Figure 8: Velocity-field characteristic for real-space transfer device with AlGaAs thickness as a parameter. All other parameters are the same as in Fig. 2.](Image)

![Figure 9: Relative occupancy of electrons in AlGaAs thickness as a parameter, as a function of electric field. All other parameters are the same as in Fig. 2.](Image)
GaAs. For all practical purposes, the resultant velocity-field characteristic would be dominated by the heavily compensated GaAs. In Fig. 7, the free-electron density is $10^{17}$ cm$^{-3}$ and the ionized impurity density is $10^{19}$ cm$^{-3}$. The results in this figure for a barrier height of 0.1 eV are consistent with these conclusions based on our own calculations on bulk, heavily compensated GaAs, and with other calculations on more heavily doped GaAs.\textsuperscript{10}

It appears that for a given materials system there will be an optimum barrier height for most effectively utilizing real-space transfer in a given device application. For the GaAs/AlGaAs system studied in this paper, a barrier height in the vicinity of 0.2 eV results in an attractive set of material parameters for consideration for negative resistance devices.

Figure 8 shows the influence of respective layer thickness on the velocity-field characteristics of the layered heterostructure. Figure 9 shows the occupancy in the AlGaAs as a function of the electric field intensity. Again, the influence of size quantization has not been included and could influence the results for GaAs layer thicknesses of 100 Å. The purpose of these last two figures is to show in a qualitative manner the way in which simple geometric changes can be used to control the transport properties of a layered heterostructure.

**IV. SUMMARY AND CONCLUSIONS**

The Monte Carlo simulations presented here have validated the general features of the phenomenon of real-space electron transfer discussed and examined by Hess and co-workers at the University of Illinois.\textsuperscript{1,4} The simulation model presented here has included the important scattering processes and energy exchange mechanisms between the two adjacent materials in layered heterostructures. It predicts that real-space transfer provides a mechanism for negative differential conductivity that is analogous to the Gunn effect, but which is different from it to the extent that the nature of the mechanism can be "engineered" by the materials and device designer. This includes the control of the important parameters such as velocity-field characteristic and speed of response. The work discussed here is now being extended to the investigation of other practical materials systems and to the inclusion of other important physical mechanisms such as size quantization, interface effects, heavy doping effects, and electron-electron interactions.

**ACKNOWLEDGMENTS**

The authors wish to thank the Department of Defense for financial support of this work through the Joint Services Electronics Program (U.S. Army, U.S. Navy, U.S. Air Force) under Contract No. N00014-79-C-0424, the Office of Naval Research under Contract Nos. N00014-76-C-0768, N00014-76-C-0806, N00014-76-C-0480, and the U.S. Army Research Office under Contract No. DAAG29-79-D-1003.

\textsuperscript{13}C. M. Wu and E. S. Yang, Solid-State Electron. 22, 241 (1979).
Measurements of hot-electron conduction and real-space transfer in GaAs-
Al,Ga, As heterojunction layers

Department of Electrical Engineering and the Coordinated Science Laboratory, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801

(Received 25 August 1980; accepted for publication 16 October 1980)

Measurements of the current-voltage characteristics of GaAs-Al,Ga, As heterojunction layers are reported. The experimental results are consistent with the idea of real-space transfer of the electrons out of the GaAs into the Al,Ga, As under high-electron conditions. Current saturation and negative differential resistance are observed as predicted by Monte Carlo simulations.

PACS numbers: 72.20.Ht, 73.40.Lq

Electronic transport in semiconductor heterojunction layers has attracted considerable interest since Dingle and co-workers verified mobility enhancement in modulation-doped structures. Such enhancement occurs when electrons leave their parent donors (e.g., in the Al,Ga, As) and transfer to a neighboring undoped layer which has a smaller band gap (e.g., GaAs). Thus the electrons will not be scattered strongly by the remote impurities (donors) and the mobility in the GaAs will be enhanced. Although there are some subtleties, including an enhanced phonon scattering rate, this improved mobility is reflected in the experiments.

Theoretical investigations of high-field transport in these layers led Hess et al. to conclude that when a high electric field is applied parallel to the layer interfaces the inverse process takes place, namely a transfer of electrons from the GaAs layers back into the Al,Ga, As layers. This process can be viewed as the thermionic emission of hot electrons, and has simple mechanical analogies. A Monte Carlo simulation of the real-space trajectory of an electron for a double heterojunction of Al,Ga, As (x = 0.17) is shown in the inset of Fig. 1. After some reflections an electron in the GaAs layer gains enough kinetic energy from the applied electric field to move out of the potential well caused by the band-gap difference between the two materials. More exact treatments of this effect including quantum-mechanical transmission coefficients do not reveal new features for this picture.

The movement of the hot electrons back into the low-mobility Al,Ga, As material will of course lead to a nonlinear behavior in the current density. Figure 1 shows the current-voltage characteristic of the double-heterojunction structure shown in the inset. These results were obtained from Monte Carlo calculations. The magnitude of the negative differential resistance in such a curve depends on the doping densities which control the free-carrier concentrations and mobilities in the Al,Ga, As and GaAs layers. A very high doping density in the Al,Ga, As causes a high concentration of scattering centers, which results in a very low mobility and high resistance in the Al,Ga, As and therefore can yield large peak-to-valley ratios, larger than those observed in the Gunn effect, which is based on the k-space analog of the mechanism described here.

In this letter we report measurements of the high-field characteristics of Al,Ga, As structures grown by molecular beam epitaxy (MBE). The doping density in the Al,Ga, As layers was \( N_d \approx 10^{17} \text{ cm}^{-2} \) and the GaAs was not intentionally doped. The mobility in the GaAs layers was enhanced over the bulk value for equivalent doping and was typically \( 2 \times 10^4 \text{ cm}^2/\text{V s} \) at 77 K. The mobility in the Al,Ga, As layers was around \( 10^5 \text{ cm}^2/\text{V s} \) at 300 and 77 K. The doped Al,Ga, As layer was 1000 Å thick in all cases, whereas the GaAs layers varied in thickness from 400 Å to \( 1.0 \mu\text{m} \). In some of the samples the GaAs layer was sandwiched between the doped and a second undoped Al,Ga, As layer. Because of the pulling force of the donors we think that the actual width of the GaAs layer is relatively unimportant, since the electrons in the GaAs will always be within 100 Å of the doped Al,Ga, As layer. Al-Ga, As contact x = 0.17 for most of the data reported here, we have made similar measurements with x increased to 0.25. Au-Ge contacts were evaporated on top of the layer (top layer Al,Ga, As) and alloyed by heating at a rate of \( 400^\circ\text{C/min} \) in flowing \( \text{H}_2 \) to a final temperature of \( 450^\circ\text{C} \). Contacts formed in this way proved to be ohmic in most cases.

The distance between the contacts was 0.065 cm and the width of the samples was about 0.1 cm. Measurements were performed using short current pulses. The measurements were taken at times between 1 and 600 ns. The samples were mounted in GR insertion units and the usual 50-Ω sampling oscilloscope-x-y recorder technique was used. Below we report five groups of results:

(i) Unusually strong acoustoelectric sound amplification and accompanying negative differential resistance (inset Fig. 2) was observed in some samples at 77 K at very low electric fields of about \( 300 \text{ V/cm} \) having incubation times as low as \( 3 \text{ ns} \). This effect did not occur at room temperature (the samples were too short) and was not observed in any of the samples for which results are reported below. A detailed report will be given in a subsequent publication.

(ii) In samples not showing the acoustoelectric effect (about 40 samples from 5 wafers) onset of current saturation or slight negative differential resistance was observed at an
electrical field of 2000–3200 V/cm at room temperature and also at 77 K. Representative examples are given in Figs. 2 and 3. The consistency of the occurrence of negative differential resistance at these fields makes us believe that contact effects do not strongly influence our experimental results.

(iii) Figure 2 also shows the onset of a second (third if the acoustoelectric effect is counted) negative differential resistance, marked by the second arrow. We believe that this may be due to trapping in surface states when electrons finally spill to the unprotected surface. The effect is apparently slow and shows hysteresis.

(iv) We performed photoconductivity measurements using the 6328-Å line of a He-Ne laser. The result exhibited by six samples is shown in Fig. 3. The low-field conductance is slightly increased by the light but the high-field conductance is strongly decreased, thus enhancing the negative differential resistance. A natural explanation is that the light empties traps in the AlGaAs, and increases the low-field conductivity. The traps are filled again when the hot electrons transfer back to the AlGaAs, thus increasing the peak-to-valley ratio of the curve and decreasing the high-field conductivity. Note also the close agreement of the dark curve in Fig. 3 with the Monte Carlo simulations of the Gunn effect in the AlGaAs, thick layer.

(v) Our knowledge of carrier concentration and mobility was obtained from Hall effect data, which reflect average concentrations and mobilities. Additional information can be obtained from the hot-electron results by assuming a value of $-10^7$ cm/s for the peak velocity. Nevertheless, the exact concentration and its spatial variation is hard to determine. Therefore, in some cases our samples showed mainly conduction in the AlGaAs, which was in these cases too highly doped to be depleted. (The built-in fields prevent complete transfer of all the electrons to the GaAs.) Some of these samples showed a fourth kind of negative differential resistance at about $10^4$ V/cm due to the Gunn effect in the AlGaAs, and also exhibited oscillations. By etching away part of the AlGaAs, depletion of the AlGaAs could be achieved, and negative differential resistance was again observed around 3000 V/cm. This experiment also gave another estimate of the doping from the known depletion width, which was obtained from the etch-
Dipole-like domains cannot be formed because accumulating electrons. A representative example is shown in Fig. 4. The effect is different from the effect of k-space transfer [the Ridley-Watkins-Hilsum (RWH) mechanism]. The distinction from the RWH effect in Al$_{x}$Ga$_{1-x}$As is demonstrated by the etching experiment of Fig. 4. Negative differential resistance due to k-space transfer in GaAs is also different from the effect described here. The threshold voltage is somewhat higher for the RWH mechanism, but this could also be caused by the higher mobility and contact effects in our samples. However, the Monte Carlo simulations show that for $x<0.17$ (where the band-gap difference is smaller than the energy separation to the satellite minima) the electrons move out of the GaAs long before they can populate higher valleys. Furthermore, the photoconductive enhancement of the negative differential resistance (Fig. 3) does not occur for the RWH effect and can not be simply explained without the transfer of electrons out of the GaAs.

We have never observed Gunn oscillations connected with the negative differential resistance at 3000 V/cm. The reason for this is not entirely understood. However, we can point out the following distinct differences between real-space transfer and the RWH mechanism. There is no local microscopic negative differential resistance in the Al$_{x}$Ga$_{1-x}$As at the electric fields considered. Accumulation (and therefore dipole) domains cannot be formed because accumulating electrons would be emitted out of the GaAs. The total lack of any kind of instability, however, does not necessarily follow from these arguments and might be connected with fixed interface inhomogeneities at which the electrons spill out first.

The speed of the effect could not be determined with the present experimental arrangement. We can only say that the effect is faster than 1 ns. Our measurements below 1 ns were hampered by parasitic capacitances possibly caused by the layered structure itself. Finally, we would like to mention that the peak-to-valley ratio of the current-voltage characteristic will depend strongly on the electron mobility of the Al$_{x}$Ga$_{1-x}$As. To obtain high peak-to-valley ratios, the mobility in the Al$_{x}$Ga$_{1-x}$As should be around 100 and $>5000$ cm$^2$/V s in the GaAs. In order to allow simultaneously for depletion of the Al$_{x}$Ga$_{1-x}$As, highly compensated material is needed. If low mobilities in compensated material can be achieved without introducing deep traps, the resulting negative differential resistance should have a peak-to-valley ratio much larger than that achievable by the RWH mechanism.

For assistance in portions of this work we wish to thank Susan Brennecke, Bob McFarlane, and R. T. Gladin. We are particularly grateful to N. Holonyak, Jr. for many valuable discussions and to A. Y. Cho for assisting the MBE program. We also thank M. A. Littlejohn, T. H. Glisson, and J. R. Hauser of North Carolina State University (Raleigh) for providing us with the Monte Carlo stimulation results. The work has been supported primarily by the Office of Naval Research, Contract No. N000-14-79-C-0768, and the Army Research Office, Contract No. DAAG-19-80-C-0011. The crystal growth facilities have been supported by the Air Force Office of Scientific Research, Contract No. AFOSR-80-0084, and the Joint Services Electronics Program, Contract No. N000-14-79-C-0429.

6. T. H. Glisson, J. R. Hauser, and M. A. Littlejohn (private communication).
Simulation of high-field transport in GaAs using a Monte Carlo method and pseudopotential band structures

H. Shichijo, K. Hess, and G. E. Stillman
Department of Electrical Engineering and Coordinated Science Laboratory, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801

(Received 15 August 1980; accepted for publication 16 October 1980)

We have performed a Monte Carlo simulation of high-field transport in GaAs using a realistic band structure obtained by the empirical pseudopotential method. On this basis, a detailed study of the band structure dependence of impact ionization in GaAs is given. Our method avoids the use of the effective mass theorem or the Kane model of nonparabolicity, which are no longer accurate at high electron energies. We show (i) that the orientation dependence of the impact ionization rate is negligibly small, (ii) that the saturation velocity of electrons in GaAs is close to \(6 \times 10^6\) cm/s at extremely high fields (this value is determined to a large extent by the band structure, and (iii) that the previous theories of impact ionization as given by Wolff, Shockley, and Baraff have numerous limitations.

PACS numbers: 72.20.Ht, 72.10.-d, 79.20.Hx, 85.30.De

Impact ionization and other high-field phenomena are of considerable interest because many semiconductor devices are based on high-field effects (avalanche photodiodes, IMPATT diodes, Gunn diodes) or necessarily involve them in their operation and are limited because of them (charge coupled devices, field effect transistors). In spite of the urgent need, a rigorous theory for electronic transport above about \(5 \times 10^4\) V/cm has not been developed. The main reason for this is that any theory applicable at high electric field must include a realistic band structure and abandon the effective mass approximation or simple extensions using the k-p method to allow for nonparabolicity.

Surprisingly enough, for specific quantities (such as the impact ionization rate) successful phenomenological theories have been given without including the band structure. These theories developed by Wolff, Shockley, Baraff, Dumke, and Chwang et al. fail, however, when used to calculate other transport quantities or when applied to different materials. Dumke's theory is only applicable to InSb or InAs, whereas Wolff's, Baraff's, and Chwang's treatments are only valid for nonpolar materials. The reason for the partial success of theories is that adjustable parameters are used, which can successfully "absorb" the band-structure effects on the field dependence of the impact ionization rate, but do not "absorb" these effects for other transport quantities. Effects of crystal orientation can not be practically treated by these theories at all. The reason is that the inclusion of the band structure in analytical solutions of the Boltzmann equation is impractical, if not impossible.

The Monte Carlo method provides an alternative to the solution of the Boltzmann equation. This method can be used to calculate the impact ionization rate, the drift velocity, and other quantities of interest without any a priori assumptions on the form of the distribution function. The Monte Carlo method can also take into account a large variety of scattering mechanisms and, therefore, is applicable to both polar and nonpolar semiconductors. In this letter we report the use of the Monte Carlo method with a realistic band structure as calculated by the empirical pseudopotential method for the calculation of high-field transport. The numerical procedure is as follows. The \(E(k)\) relation and its gradients (velocity) have been calculated using the 48-fold symmetry of the Brillouin zone (156 mesh points in the \(1/48\) part of the zone). The \(E(k)\) relation for an arbitrary \(k\) vector...
FIG. 1. Typical trajectory of the electron k vector in the Brillouin zone for an electric field of 500 kV/cm. The solid lines represent the drifts and the broken lines represent the scatterings from one point to the next.

FIG. 2. Calculated electric field dependence of the electron initiated impact ionization rate in GaAs. The shaded region indicates the range of available experimental data. (See Refs. 17 and 18.)

FIG. 3. Calculated electron drift velocity in GaAs at room temperature compared with the experimental data. (See Refs. 19 and 20.)

The impact ionizing collision is treated as an additional scattering mechanism. We assume an isotropic threshold energy of 2.0 eV. According to Keldysh, the probability of impact ionization can be represented as

$$\frac{1}{\tau(E)} = \frac{1}{\tau(E_i)} \rho \left( \frac{E - E_i}{E_i} \right)^2,$$

where $E$ is the electron energy, $E_i$ is the threshold energy, $1/\tau(E_i)$ is the scattering rate at $E = E_i$, and $\rho$ is a dimensionless constant which is generally much larger than unity. This formula is valid for semiconductors with large dielectric constants. We insert $\rho = 400$. A more rigorous treatment must involve the calculation of the matrix element for the screened Coulomb interaction.

The simulation then starts by releasing an electron with zero energy at the bottom of the central valley. The motion of an electron during the drift is determined by the equations of motion.

rate in the satellite valleys), the overestimation is at least partly compensated.

The final state of the scattering process is determined in the following way. Since polar optical scattering is dominant only at low energies in the central valley, the usual formula with effective mass and nonparabolicity terms is used to choose a candidate for the final k point. The energy at this k point is then recalculated using the exact band structure to check if it is within an allowed range (~30 meV) around the final energy $(E + \hbar \omega_k)$ in the case of phonon absorption. If it is outside this range, a different final state is chosen, and the process is repeated until a proper state with correct energy is found. Intervalley scattering is known to be completely randomizing. For this mechanism, once the final energy is calculated, those mesh points, whose energies are within the allowed range, are tabulated. One of them is then randomly selected as the final state.

Our treatment of phonon scattering processes represents a compromise between accuracy and numerical tractability. In the limit of infinitely fine mesh points (instead of 156 points in 1/48 of the Brillouin zone) and infinitely small allowed final energy range (instead of 30 meV) the procedure is basically correct as the scattering rate for deformation potential scattering is proportional to the final density of states.

The impact ionizing collision is treated as an additional scattering mechanism. We assume an isotropic threshold energy of 2.0 eV. According to Keldysh, the probability of impact ionization can be represented as

$$\frac{1}{\tau(E)} = \frac{1}{\tau(E_i)} \rho \left( \frac{E - E_i}{E_i} \right)^2,$$

where $E$ is the electron energy, $E_i$ is the threshold energy, $1/\tau(E_i)$ is the scattering rate at $E = E_i$, and $\rho$ is a dimensionless constant which is generally much larger than unity. This formula is valid for semiconductors with large dielectric constants. We insert $\rho = 400$. A more rigorous treatment must involve the calculation of the matrix element for the screened Coulomb interaction.

The simulation then starts by releasing an electron with zero energy at the bottom of the central valley. The motion of an electron during the drift is determined by the equations of motion.

rate in the satellite valleys), the overestimation is at least partly compensated.

The final state of the scattering process is determined in the following way. Since polar optical scattering is dominant only at low energies in the central valley, the usual formula with effective mass and nonparabolicity terms is used to choose a candidate for the final k point. The energy at this k point is then recalculated using the exact band structure to check if it is within an allowed range (~30 meV) around the final energy $(E + \hbar \omega_k)$ in the case of phonon absorption. If it is outside this range, a different final state is chosen, and the process is repeated until a proper state with correct energy is found. Intervalley scattering is known to be completely randomizing. For this mechanism, once the final energy is calculated, those mesh points, whose energies are within the allowed range, are tabulated. One of them is then randomly selected as the final state.

Our treatment of phonon scattering processes represents a compromise between accuracy and numerical tractability. In the limit of infinitely fine mesh points (instead of 156 points in 1/48 of the Brillouin zone) and infinitely small allowed final energy range (instead of 30 meV) the procedure is basically correct as the scattering rate for deformation potential scattering is proportional to the final density of states.

The impact ionizing collision is treated as an additional scattering mechanism. We assume an isotropic threshold energy of 2.0 eV. According to Keldysh, the probability of impact ionization can be represented as

$$\frac{1}{\tau(E)} = \frac{1}{\tau(E_i)} \rho \left( \frac{E - E_i}{E_i} \right)^2,$$

where $E$ is the electron energy, $E_i$ is the threshold energy, $1/\tau(E_i)$ is the scattering rate at $E = E_i$, and $\rho$ is a dimensionless constant which is generally much larger than unity. This formula is valid for semiconductors with large dielectric constants. We insert $\rho = 400$. A more rigorous treatment must involve the calculation of the matrix element for the screened Coulomb interaction.

The simulation then starts by releasing an electron with zero energy at the bottom of the central valley. The motion of an electron during the drift is determined by the equations of motion.
\[
\frac{dke}{dt} = eF,
\]

\[
v = \frac{1}{k} \nabla_x E,
\]

where \( F \) is an electric field vector, and \( v \) is the electron velocity in real space. The drift time and the scattering events are determined by random numbers as in conventional Monte Carlo methods. When impact ionization occurs, the energy of an electron is reinitialized to zero. The impact ionization rate can be obtained by averaging the distance to impact ionization over a sufficient number of ionizations. Each distance traveled during the drift is calculated either by accumulating a differential distance, \( \Delta x \), or by utilizing the relation

\[
\Delta E = eF\Delta x,
\]

where \( \Delta E \) is the energy gained during the drift.

Figure 1 shows a typical trajectory of the \( k \) vector in the Brillouin zone for an electric field of 500 kV/cm in the \((100)\) direction. The solid lines represent the drift of the electron, and the broken lines represent the scatterings from one point to another. When the \( k \) vector lies outside of the Brillouin zone, it is placed back to the equivalent point inside the zone. A typical simulation consists of approximately 100,000–200,000 scattering events.

The calculated electric field dependence of the impact ionization rate in GaAs is shown in Fig. 2. The shaded region indicates the range covered by the currently available experimental data. The agreement is fairly good considering the uncertainty in the scattering rate at higher energies. The inclusion of upper bands is expected to increase the calculated ionization rate slightly. Within statistical fluctuations (\( \sim 20\% \)) we do not see any orientation dependences of the ionization rate. This contradicts the experimental data by Pearsall et al., who found that the ionization rate differs in various crystal directions by almost an order of magnitude at lower fields.

Figure 3 shows the electron drift velocity in GaAs calculated by our method. The broken curve represents the experimental data. The agreement is good in the whole range of electric fields which has been investigated experimentally. The slight deviations between theory and experiment are believed to be mainly due to the pseudopotential band structure which gives the effective masses at the \( \Gamma \), \( X \), and \( L \) valleys larger than are usually measured. In Fig. 3 it can also be seen that the calculations describe quantitatively the Gunn effect. Both \( X \) and \( L \) valleys are of course automatically included.

These are three major results which have been obtained with one set of material constants. We now describe briefly some other results of more qualitative nature. We have learned that the electrons are not at all drifting mainly in the direction of the electric field; they are frequently scattered practically all over the Brillouin zone (Fig. 1). The electrons move over relatively long time periods perpendicular to the external fields because of Bragg reflection at energies above 1 eV. Moreover, we find hardly any "lucky" electrons which totally escape the phonon scattering. This contradicts some of Shockley's ideas of impact ionization. Shockley's "lucky" electrons start from zero energy, escape the phonon scattering, and impact ionize. We find instead that the electrons stay around an average energy of typically 0.8 eV (for the case of 500 kV/cm) and experience a large number of scattering events. Once in a while electrons escape the phonon scattering events and move up to higher energy. Then if they are lucky enough they reach ionization threshold after a few (typically three to five) scattering events. In view of these facts the question arises why the previous theories of impact ionization are so successful and which one is the closest to the truth? For instance, Shockley's physical arguments linking the number of phonon scatterings and the probability to impact ionize are reflected also by our simulations. The quantitative success of previous theories, however, is connected with the large number of adjustable parameters.

Our method can, of course, be applied to any semiconductor. The calculations, however, can be costly and time consuming. The above simulation takes about an hour of CPU time on a DEC-20 for each value of the electric field. However, the efficiency of the program has not yet been optimized. Finally, we would like to note that the problem of hot electron emission from silicon into silicon dioxide \(^{21} \) over a potential barrier of \( \sim 3 \) eV certainly needs the inclusion of a realistic band structure. Calculations on this problem are in progress.

We would like to thank N. Alparelli for his help with the band-structure calculations. This work was supported by the Office of Naval Research under Contract No. N00014-79-C-0768 and the Joint Services Electronics Program under Contract No. N00014-79-C-0424. The use of the computer facilities of the Materials Research Laboratory, University of Illinois, under Contract No. DMR 77-23999 is also gratefully acknowledged.

Band-structure-dependent transport and impact ionization in GaAs

H. Shichijo and K. Hess
Department of Electrical Engineering and Coordinated Science Laboratory,
University of Illinois at Urbana-Champaign, Urbana, Illinois 61801
(Received 14 October 1980)

We have performed a Monte Carlo simulation of high-field transport in GaAs including a
realistic band structure to study the band-structure dependence of electron transport and impact
ionization. The band structure has been calculated using the empirical pseudopotential method.
Unlike previous theories of impact ionization, our method is capable of calculating various
parameters, such as mean free path, from first principles. The calculated electron mean free path,
drift velocity, and impact ionization rate are in reasonable agreement with the experimen-
tal data in spite of several simplifications of the model. Within statistical uncertainty we do not
observe any orientation dependence of the ionization rate in contradiction to the interpreta-
tion of recently reported experimental results. We also find that the contribution of ballistic
electrons to impact ionization is negligibly small. Based on the results of the calculation, a general
discussion of impact ionization is given.

I. INTRODUCTION

A large number of semiconductor devices operate
on the basis of highly energetic (hot) electrons. Im-
 pact ionization is an essential mechanism in the
operation of photodetectors and impact-avalanche
diode (IMPATT) diodes. At present, however,
the understanding of this effect is limited to a
number of theories which contain several adju-
sable parameters whose physical significance is not
well understood. The most widely used theory of im-
 pact ionization has been given by Baraff. The
adjustable parameters of his theory are the threshold
energy for ionization, the optical-phonon energy, the
ionization mean free path, and the mean free path
for optical-phonon scattering. Although some at-
ttempts have been made to determine these parameters theoretically, a “complete”
theory of impact ionization, which is capable of calculat-
ing these quantities (and therefore the ionization
rate) from first principles, has not been developed.
The main reason is that any theory applicable at ex-
tremely high electric fields (causing ionization) must
abandon the effective-mass approximation or simple
extensions using the K-β method, and instead in-
clude a realistic band structure. The surprising suc-
cess of Baraff’s theory in explaining the electric field
dependence of the ionization rate is due to the adju-
sable parameters, which can “absorb” the band-
structure effects. The inclusion of the band structure
in solutions of the Boltzmann equation, however, is
impractical. It is also difficult to include realistic
scattering mechanisms. For example, the inclusion
of both small angle scattering and randomizing
scattering mechanisms in the same analytical frame-
work is difficult. As a consequence all the previous
theories are only applicable to specific materials. For
instance, Dumke’s theory is only applicable to InSb
or InAs, whereas Baraff’s or the Chwang et al...
sight into how the various parameters in previous theories are connected and into how the band structure influences the impact ionization rate. In particular, the method is applied to study the electron-initiated ionization in GaAs. The results also give us information about the accuracy of the pseudopotential band structure at high energies.

II. SUMMARY OF EXPERIMENTAL RESULTS

Before we discuss the theory of impact ionization, it is instructive to summarize the available experimental data. Various experimental techniques to measure the ionization rate are described in detail in the review paper by Stillman and Wolfe.1 Their article also contains some of the experimental data on the electron-initiated ionization rate in GaAs. Figure 1 summarizes more recent data.6-19 The experimental results usually show a $1/F^2$ dependence of the ionization rate ($F$ is the electric field). As can be seen from the figure, the data of different workers scatter almost by an order of magnitude.

Of special interest are the results of Pearsall et al.,19 who measured the electron ionization rate with the electric field applied in three different crystallographic directions. Their data are replotted in Fig. 2. They have measured the highest ionization rate in the (110) direction and the lowest in the (111) direction. They have attributed this difference to ballistic electrons and electron tunneling to the next higher conduction band.18,20 Although these data raise an interesting question as to how the band structure actually influences the ionization rate, their notion of ballistic electrons seems to be incorrect, as is shown in this work. More systematic and reliable data are necessary to make a comparison with the theory.

III. PREVIOUS THEORIES OF IMPACT IONIZATION

Wolff1 was the first to calculate the ionization rate in semiconductors. He applied the gas discharge theory to solve the Boltzmann equation taking into account the effect of electron-phonon and pair-producing collisions on the distribution function. The velocity distribution function was approximated as

$$n(v, \theta) = n_0(v) + n_1(v) \cos \theta.$$  

(1)

where $v$ is the electron velocity, and $\theta$ is the angle between the velocity and the electric field. This is an energy diffusion theory, in which the electrons undergo many collisions when moving to higher energies. The Boltzmann equation was then solved to calculate the ionization rate with the result

$$\alpha(F) = \exp(-A/F^2).$$  

(2)

where $F$ is the electric field.

Shockley,4 on the other hand, argued that ionization is mainly due to "lucky" electrons which completely escape phonon scatterings and reach the threshold energy. In this streaming approximation the distribution is a spike in the direction of the electric field. He considered the relative probability of
phonon scattering and pair production, and obtained an ionization rate whose dependence on $F$ is given by

$$\alpha(F) = \exp(-B/F) \quad (3)$$

Next, Baraff\textsuperscript{3, 4} solve the time-independent Boltzmann equation and showed that his result contained Shockley's result as a low-field limit, and Wolff's result as a high-field limit. His theory gives the "universal" curves with phonon mean free path and ionization threshold energy as parameters, which are adjusted to fit theory to experimental data. However, it does not provide a way to calculate these quantities, nor does it include the band structure.

Recently, Chwang et al.\textsuperscript{5} took a different approach using a finite Markov chain formulation. Their method is based on the calculation of a transition matrix which characterizes the transition probability between virtual states defined by small discrete energy intervals. Interesting as it is, their method is limited for the interpolation of energy in the proximity of the analytical formulations. It still requires the same assumptions as Baraff's theory and does not produce much more information. For example, an assumption of a constant mean free path for phonon scattering is still necessary. Moreover, the Markov formulation is only applicable to nonpolar semiconductors.

Nevertheless, Baraff's and Chwang's theories contain some "truth" about the impact ionization mechanism, as does Shockley's and Wolff's approach. How they are related, and how they complement each other will be clear as a result of the Monte Carlo calculation described in this work. This Monte Carlo method includes a realistic band structure. As a result, the orientation dependence of the impact ionization can also be calculated.

### IV. BAND STRUCTURE OF GaAs

The band structure of GaAs has been calculated using the empirical pseudopotential method as described by Cohen and Bergstresser.\textsuperscript{15} Only the lowest conduction band has been considered. The effect of higher bands is briefly discussed in the later sections. Advantage is taken of the 48-fold symmetry of the Brillouin zone of the zinc-blende structure.\textsuperscript{22} It is only necessary to examine a $\frac{1}{24}$th of the zone. This region is defined by the conditions

$$0 \leq k_x, k_y, k_z \leq \frac{\pi}{a} \quad (4)$$

and

$$k_x + k_y + k_z \leq \frac{\pi}{2} \quad (5)$$

where all the $k$ components are in units of $2\pi/a$ ($a$ is the lattice constant, $a = 5.64 \text{ Å}$ for GaAs). Mesh points ($k_x, k_y, k_z = 0.0.0.1, \ldots$) are sampled from this region, and the energy and its gradient (velocity) at each $k$ point are calculated. A total of 249 points have been sampled with 156 points within the region. The extra 93 points outside the region are necessary for the interpolation of energy in the proximity of the surface of the sampling region. Figure 4 illustrates the isoenergy lines in the cross section of the Brillouin zone shown in Fig. 3, with the numbers representing the electron energy from the bottom of the conduction band (at $\Gamma$). It can be seen that the $\Gamma$ valley is nearly isotropic, whereas the $X$ valleys are more elliptic. The band structure is then stored in memory, and used in the Monte Carlo simulation which is described in Sec. VI.

For the study of "lucky electron" transport extra $k$ points have been sampled in three major crystal directions, i.e., the (100), (110), and (111) directions. The results have made it obvious (see, for example, Fig. 5 of Ref. 15) that the use of the effective mass and nonparabolicity is not valid for electron energies above approximately 1 eV in some directions. In fact, the effective mass defined as

$$\frac{1}{m^*} = \frac{1}{\hbar^2} \frac{\partial^2 E(k)}{\partial k^2} \quad (6)$$

goes to negative values at higher energies.

---

**FIG. 3.** Cross section of the Brillouin zone.

**FIG. 4.** Isoenergy lines of the lowest conduction band of GaAs in the cross section shown in Fig. 3. The numbers represent the energies measured from the $\Gamma$ minimum.
V. BALLISTIC ELECTRON TRANSPORT AND PHONON SCATTERING

The term "ballistic electrons" has recently been used to denote those electrons which do not suffer phonon scattering.\textsuperscript{20,21} This is equivalent to the "lucky" electron notion in Shockley's theory. Since the possible contribution of ballistic electrons to impact ionization has been suggested,\textsuperscript{22} the behavior of ballistic electrons has been examined using the pseudopotential band structure. The study has been performed by solving the equations of motion

\[ \frac{d\mathbf{k}}{dt} = e\mathbf{F} \]  \hspace{1cm} (7)

and

\[ \mathbf{v} = \frac{1}{\hbar} \nabla E(\mathbf{k}) \]  \hspace{1cm} (8)

where \( \mathbf{F} \) is the applied electric field, \( \mathbf{k} \) is the electron wave vector, \( E \) is the electron energy, and \( \mathbf{v} \) is the group velocity of the electron. Equations (7) and (8) are solved simultaneously with the initial condition \( \mathbf{k} = 0 \) at \( t = 0 \), to express \( \mathbf{v} \) and \( E \) as a function of time \( t \). The field is assumed to be constant. Results of the calculations are shown in Fig. 5 for the three major crystallographic directions. The electric field has been chosen to be 500 kV/cm, a typical field for impact ionization. Figure 5 shows the electron velocity, \( \mathbf{v} \), as a function of time. The orientation dependence of the ballistic behavior is obvious from this figure. The highest peak velocity is reached in the (100) direction (\( \sim 1.1 \times 10^8 \) cm/sec) and the lowest in the (111) direction (\( \sim 0.8 \times 10^8 \) cm/sec).

In a nonideal crystal, however, ballistic transport must compete with scattering processes. It will be shown by the Monte Carlo simulation that on the average an electron can travel ballistically for only \( \sim 3 \times 10^{-10} \) sec before it suffers a phonon scattering. In the (111) direction, the electron can never gain sufficient energy ballistically for impact ionization.\textsuperscript{19} In the (100) direction, the impact ionization threshold can be reached only if electrons tunnel in \( k \) space to the next higher band \( \epsilon = 0.2 \) eV above the principal conduction band.\textsuperscript{18,19} Therefore scattering events be-

\[ \text{FIG. 5} \] Variation of ballistic electron velocity with time in three crystallographic directions of GaAs.

\[ \text{FIG. 6} \] (a) Example of wave-vector trajectory of electron in \( \Gamma KL \) plane under the influence of electric field in the (111) direction. Electron is scattered from \( A \) to \( B \). Energy change in the scattering process has been neglected. (b) Variation with time of electron energy for the process shown in (a).
come crucial for the occurrence of impact ionization in these directions.

Electrons can be scattered in other regions of the Brillouin zone with a single scattering event being sufficient to permit the electrons to reach threshold energy. This mechanism is illustrated in Fig. 6 for an electric field applied in the $\langle 111 \rangle$ direction. An electron starts at the $\Gamma$ point and moves along the $\langle 111 \rangle$ direction. At point $A(k = (\pi/a)(0.3.0.3.0.3))$, the energy is at the maximum for this direction, but it is still much less than the threshold energy. Subsequently, the electron can be scattered (by a phonon or impurity) to some other point in the Brillouin zone, point $B$, for example. Following this scattering event, the $\langle 111 \rangle$ component of the electron wave vector continues to increase. However, the wave vector points in a direction different from the $\langle 111 \rangle$ so that the electron can now reach a higher energy. As shown in Fig. 6, the electron can actually exceed the threshold energy for impact ionization ($-2.0 \text{eV}$).

This is, of course, only one example of an electron trajectory to show the importance of scattering processes to impact ionization. The actual calculation of the impact ionization rate must involve averaging of the possible electron trajectories until the electron reaches the threshold energy. This is achieved by the Monte Carlo method which is described in the next section.

VI. SIMULATION METHOD

The Monte Carlo simulation keeps track of an electron $\mathbf{k}$ vector in the Brillouin zone until it reaches the threshold energy for impact ionization. This is done with knowledge of scattering mechanisms, scattering rates, and band structure in the whole Brillouin zone. The $E(\mathbf{k})$ relation for an arbitrary $\mathbf{k}$ point can be calculated in the following way. First, the $\mathbf{k}$ point is mapped into the sampling region by using the point-group symmetry. The energy is then calculated by quadratic interpolation utilizing the energies and the gradients of the surrounding eight mesh points. The gradient is interpolated only linearly. Applying the inverse operations on the calculated energy and gradient gives the $E(\mathbf{k})$ relation and the gradient at the original $\mathbf{k}$ point.

Next we need to know the phonon scattering rate. Ideally the scattering rate should be calculated at each $\mathbf{k}$ point in order to take into account the overlap integral. Also, when the initial or final electron state is not on the symmetry points, the selection rules become less restrictive and this may give rise to additional scattering. Moreover, even near the bottom of the valleys, it is known that the scattering rates are different in the $\Gamma$, L, and X valleys. We have assumed the scattering rate to be isotropic (only energy dependent) for simplicity and because of lack of additional information. We have taken the scattering rate as given for the central valley. This overestimates the scattering rate when the electron is in the satellite valleys. The simplification is partly justified by the fact that the scattering rates of different valleys approach each other at higher energies. Furthermore, since scattering to upper bands is possible in reality (which increases the scattering rate in the satellite valleys), the overestimation is at least partly compensated.

The values of the parameters for the calculation of the scattering rate are the same as the ones used in the simulation of the Gunn effect. They are known to give a good fit to the experimental data at low fields. Below 0.33 eV only polar optical scattering occurs in the central valley. Above 0.33 eV polar optical scattering occurs only when an electron is in the central valley arbitrarily defined as

$$-0.3 \leq k_x, k_y, k_z \leq 0.3,$$

where the components are in units of $2\pi/a$. Otherwise intervalley scattering occurs. It is not appropriate to simply extend the scattering rate to higher energies because of the complicated band structure. Because the intervalley scattering rate is proportional to the density of final states, and the density of states in the conduction band decreases nearly quadratically above 1.5 eV, we have assumed a quadratically decreasing scattering rate above 1.5 eV. The resultant total scattering rate as a function of electron energy is shown in Fig. 7 (solid line). The maximum scattering rate is $4.5 \times 10^{14} \text{sec}^{-1}$ at 1.5 eV.

In the $\langle 100 \rangle$ direction the threshold state for electron-initiated ionization lies in the second conduction band. An electron can tunnel through the "pseudogap" ($-0.2 \text{eV}$) between the lowest and the second conduction band to reach threshold. No attempt has been made to simulate this tunneling mechanism. Since the tunneling time is estimated to be of the order of $1 \times 10^{-13} \text{sec}$, and the intervalley scattering time for an electron energy of 2.0 eV is much shorter ($< 1 \times 10^{-14} \text{sec}$) than this tunneling time, electrons are more likely to be scattered before they can tunnel to the upper band. Therefore, the contribution of these tunneling electrons to impact ionization is expected to be small.

The final state of the scattering process is determined in the following way. Since polar optical scattering is dominant only at low energies in the central valley, the usual formula with effective mass and nonparabolicity terms is used to choose a candidate for the final $\mathbf{k}$ point. The energy at this $\mathbf{k}$ point is then recalculated using the exact band structure to check if it is within an allowed range (typically 30 meV) around the final energy (for example, $E + E_{\text{phon}}$ in the case of phonon absorption). If it is outside this range, a different final state is chosen and the process is repeated until a proper state within the correct energy range is found. Intervalley scattering
loss is checked and ensured in our procedure. The selected as the final state. The correct overall energy is known to be completely proportional to the final density of states.

The scattering rate for deformation potential scattering of infinitely fine mesh our procedure is correct, since dependence on the final energy is calculated, those complicated E(k) relation.

By terminating the simulation after the first scattering the electron suffers, the behavior of ballistic elec-

![Phonon Scattering

FIG. 7. Phonon scattering rate and the impact ionization probability in GaAs as a function of electron energy. The parameters are due to Littlejohn et al. (solid line) (Ref. 26) and Vinson et al. (broken line) (Ref. 33).]

is known to be completely randomizing. For this mechanism, once the final energy is calculated, those mesh points whose energies are within the allowed range are tabulated. One of them is then randomly selected as the final state. The correct overall energy loss is checked and ensured in our procedure.

Our treatment of phonon scattering processes represents a compromise between accuracy and numerical tractability. For a finite number of mesh points, the energy separation between any two K points is finite. For example, for our 156 mesh points this energy separation can be as large as 60 meV. The allowed energy range during the scattering must be large enough to bridge this gap in order to assure the continuity of the energy band. In the limit of infinitely fine mesh points, the allowed range for final energy can be infinitely small. The number of K points in this energy range for a given final energy is proportional to the density of states at each region of K space with this final energy. Therefore, in the limit of infinitely fine mesh our procedure is correct, since the scattering rate for deformation potential scattering is proportional to the final density of states.

The impact ionizing collision is treated as an additional scattering mechanism. We assume an isotropic threshold energy of 2.0 eV. Anderson and Crowell have shown that the threshold energy actually depends on the K vector. However, their graphical procedure is almost impossible to perform in three-dimensional momentum space. A more systematic approach may be possible. If the threshold energy is calculated for each K point, it can be easily included in this simulation procedure. The impact ionization probability can be calculated from the matrix element for the screened Coulomb interaction. However, here we use a simpler model demonstrated by Keldysh and used by others. According to Keldysh the probability of impact ionization can be represented as

$$\frac{1}{\tau(E)} = \frac{1}{\tau(E_0)} P \left( \frac{E - E_0}{E_0} \right)^2,$$  

(10)

where E is the electron energy, E is the threshold energy, 1/\(\tau(E)\) is the scattering rate at \(E = E_0\), and \(P\) is a dimensionless constant which is usually much larger than unity. This formula is valid for semiconductors with large dielectric constants. We take \(P\) as a parameter. \(P = -50\) has been used by Chwang et al. As shown by Baraff and then by Chwang the impact ionization rate does not strongly depend on this parameter as long as \(P\) is large compared to unity. The energy dependence of the impact ionization probability for \(P = 400\) is illustrated in Fig. 7.

Once the scattering rate and the ionization probability are determined, the rest of the simulation procedure is similar to the conventional Monte Carlo method. The scattering probability \(I_i(\tau(E))\) is calculated at each time interval, \(\Delta t\), and compared with a random number. This is necessary because of the complicated \(E(\vec{k})\) relation. \(\Delta t\) is taken to be approximately \(1/10\) with the average drift time. The simulation starts by releasing an electron with zero energy at the bottom of the central valley. The energy and the K vector of the electron are traced. When impact ionization occurs, the energy is reinitialized to zero to start a new history. This is justified by the fact that the resultant electron after ionization lies very close to the bottom of the central valley. The impact ionization rate can be obtained by averaging each distance that an electron travels until impact ionization occurs over a sufficient number of ionizations. The distance, \(\Delta x\), traveled during each drift is calculated either by accumulating a differential distance, \(\nu \Delta t\), or by utilizing the relation

$$\Delta E = eF\Delta x,$$  

(11)

where \(\Delta E\) is the energy gained during the drift. The velocity \(\nu\) is calculated from the gradient of the \(E(\vec{k})\) relation.

VII. RESULTS

A. Contribution of ballistic electrons

By terminating the simulation after the first scattering the electron suffers, the behavior of ballistic elec-
tron can be studied. Additionally, we can determine the extent which these ballistic electrons contribute to impact ionization. Since there is no electron-initiated threshold state in the (100) or the (111) direction, we only consider the (110) direction. We have also changed the threshold energy to 1.7 eV, which is the correct threshold energy in this direction. Typically 100,000 trials have been done for each electric field.

The result of the calculation shows that an electron travels on the average approximately 200 Å, for an average time of $3 \times 10^{-14}$ sec before the first scattering event. These numbers differ slightly for different orientations. By counting those electrons which cause impact ionization instead of scattering, we can estimate the contribution of ballistic electrons to the impact ionization rate. If the same scattering rate is used as shown in Fig. 7 (known to give a good fit to the Gunn effect), we find no electrons (less than 0.001%) causing impact ionization. There may be some uncertainties in the scattering rate, particularly in the values of the deformation potential constants. To find the maximum possible contribution of ballistic electrons to impact ionization, a smaller scattering rate has been tried. We have used the values given by Vinson et al.: $E_{F-L} = 0.4$, $E_{F-C} = 0.38$ eV, $D_{F-L} = 1.1 \times 10^9$, and $D_{F-C} = 2.8 \times 10^9$ eV/cm. This gives the scattering rate shown by the broken line in Fig. 7. This rate is approximately half of the previous value. Using this scattering rate in our calculation we obtain the results shown in Fig. 8. This figure shows the probability that an electron causes impact ionization prior to its scattering by a phonon as a function of electric field. As can be seen, even at the maximum (500 kV/cm for $P = \infty$), only 0.2% of the electrons causing impact ionization are "ballistic." Therefore we conclude that the contribution of ballistic electrons to impact ionization is negligibly small if our present understanding of the scattering rate is correct. This conclusion negates the considerations by Capasso et al. who suggested that ballistic electrons give a non-negligible contribution to the total ionization rate.

These "ballistic" electrons were discussed by Shockley who called them "lucky" electrons. We have shown that Shockley's theory gives ionization rates that are too small. It is interesting to note, however, that the two curves in Fig. 8 show the correct $1/F$ dependence as in Shockley's theory in spite of the much more complicated band structure and scattering rate that we used.

B. Transport properties and ionization rate

In the calculation of the impact ionization rate a typical simulation consists of approximately 200,000 to 400,000 scattering events. Depending on electric field this would give 40–300 impact ionization events. Figure 9 shows a typical trajectory of the $k$ vector in the Brillouin zone for an electric field of 500 kV/cm in the (100) direction. The solid lines represent the drift of the electron, and the broken lines represent the scatterings from one end to the next. When the $k$ comes to lie outside of the Brillouin zone, it is placed back inside the zone to the equivalent point. This is done by adding the appropri-
FIG. 10. Impact ionization rate in GaAs as a function of the number of ionizations obtained with the Monte Carlo simulation. The calculation is from the slope of the $E(k)$ curve (A) or from Eq. (11) (O).

FIG. 11. Average electron energy in GaAs as a function of electron field calculated by the Monte Carlo simulation.

FIG. 12. Electron mean free path in GaAs as a function of electric field calculated by the Monte Carlo simulation (steady state).

FIG. 13. Calculated electron drift velocity in GaAs at room temperature compared with the experimental data (Refs. 36 and 37). The calculated values are from the slope of the $E(k)$ curve (A) or from Eq. (11) (O).

The calculated electric field dependence of the electron drift velocity is shown in Fig. 13. The broken curve represents the experimental data by Ruch and Kino at low electric field ($<14$ kV/cm), and by Houston and Evans at high field ($-20$ to $100$ kV/cm). The agreement is good over the entire range of electric fields experimentally investigated.

The result using Eq. (11) gives much better fit than the result using the slopes of the $E(k)$ relation. It is agreement with previous data and the conventional Monte Carlo calculation. The reason that our calculation agrees in this respect with the conventional interpretation which does not include a realistic band structure is that the mean free path is mainly determined by the average electron energy, which is still small enough ($\approx 0.8$ eV) for effective mass and nonparabolicity corrections to be sufficient (at least in certain $k$ directions).

The electron is frequently scattered over practically the entire Brillouin zone. As seen from the figure the drift time is very short because of the high scattering rate at higher energies. The calculation is from the slope of the statistical fluctuation is estimated to be approximately 20%. The problem of statistical fluctuation can be overcome by repeating the simulation only for the high-energy tail. This has not been attempted in this work.

Figure 11 shows how the calculated ionization rate converges as the number of ionizations is increased. Because of the limited computer time it has not been possible to take averages over more than 300 ionizations. However, the convergence is fairly good after 10 ionizations. From this figure the statistical fluctuation is estimated to be approximately 20%. The electron is frequently scattered over practically the entire Brillouin zone.

Figure 10 shows how the calculated ionization rate converges as the number of ionizations is increased. Because of the limited computer time it has not been possible to take averages over more than 300 ionizations. However, the convergence is fairly good after 10 ionizations. From this figure the statistical fluctuation is estimated to be approximately 20%. The problem of statistical fluctuation can be overcome by repeating the simulation only for the high-energy tail. This has not been attempted in this work.

Figure 11 shows how the calculated ionization rate converges as the number of ionizations is increased. Because of the limited computer time it has not been possible to take averages over more than 300 ionizations. However, the convergence is fairly good after 10 ionizations. From this figure the statistical fluctuation is estimated to be approximately 20%. The problem of statistical fluctuation can be overcome by repeating the simulation only for the high-energy tail. This has not been attempted in this work.

Figure 11 shows how the calculated ionization rate converges as the number of ionizations is increased. Because of the limited computer time it has not been possible to take averages over more than 300 ionizations. However, the convergence is fairly good after 10 ionizations. From this figure the statistical fluctuation is estimated to be approximately 20%. The problem of statistical fluctuation can be overcome by repeating the simulation only for the high-energy tail. This has not been attempted in this work.
suspected that the accumulation of numerical errors in the slope calculation is responsible for the discrepancy. The slight deviations between theory and experiment at higher fields are believed to be mainly due to the pseudopotential band structure which gives the satellite valley effective masses larger than are usually assumed. From Fig. 13 it can also be seen that the calculations describe quantitatively the Gunn effect. This means that the method can simulate polar optical scattering as well as intervalley scattering, and that the transition from polar optical (low-energy region) to intervalley scattering (high-energy region) is accomplished smoothly.

Figure 14 shows the calculated electric field dependence of the impact ionization rate in GaAs for three different crystal orientations. We have assumed $P = 400$. The shaded region indicates the range covered by the experimental data (Sec. II). The agreement is fair, considering the uncertainty in the scattering rate at higher energies. The inclusion of upper bands is expected to increase the calculated ionization rate slightly, and therefore to improve the fit to the experimental data. Note, however, that the calculation shows within statistical uncertainty ($\sim 20\%$) no orientation dependence for the ionization rate. This contradicts previous interpretations of the experimental data by Pearsall et al.\(^5\) (Fig. 2).

Another way to calculate the orientation dependence is rotating the electric field direction from one axis to another. The result is shown in Fig. 15 for an electric field of 400 kV/cm when the field is rotated from the $<110>$ to $<111>$ direction. Again we do not see any orientation dependence within the statistical uncertainty. A solution including this rotation of the electric field can be obtained only by the Monte Carlo method. The effect of changing the value of $P$ has also been examined. Varying $P$ from 50 to 400 we have obtained practically the same impact ionization rate. This confirms the result by Baraff\(^5\) and Chwang\(^6\) that the ionization rate is insensitive to the orientation probability as long as it is much larger than the probability of phonon scattering.

For a better understanding of how the electrons acquire the high energies, and how impact ionization is actually accomplished, we show in Figs. 16 and 17 the variation of electron energy after each scattering event for electric fields of 500 and 100 kV/cm, respectively. In the case of 500 kV/cm, the electron energy stays around $-0.7-1.2$ eV most of the time, but the electron occasionally escapes phonon scattering and moves up to higher energies. In Fig. 16 we can see $\sim 4-5$ spikes which reach to $\sim 1.8$ eV. When an electron reaches 2.0 eV, it causes impact ionization. We can think of these electrons as the "lucky electrons" in Shockley's theory, and those electrons around the average energy as the diffusing (in energy) electrons in Wolff's theory. However, as seen in the figure this classification is not very distinct. Even those electrons in the spikes suffer several scatterings before they reach the peak energies. Our results, therefore, contain Shockley's and Wolff's notions of ionizing electrons as does Baraff's theory (but we have much more general conditions). Using Baraff's word,\(^7\) the notion of ballistic electrons by Shockley and diffusing electrons by Wolff are "complementary" in
VIII. CONCLUSIONS

A Monte Carlo simulation of high-field transport in GaAs employing a realistic band structure has been described. The method has been used to study the impact ionization mechanism in GaAs. The band structure of GaAs has been calculated using the empirical pseudopotential method. Partly due to lack of information and partly for simplicity, we have used simplifying assumptions for the phonon scattering rates, the ionization threshold energy, and the ionization probability. This, however, is not an inherent limitation of the method. Unlike previous theories of impact ionization, the method requires, in principle, no adjustable parameters as long as the band structure and the scattering mechanism are known. The method has provided new results and increased the understanding of high-field transport and impact ionization in GaAs. The calculated drift velocity, the mean free path, and the impact ionization rate are in fair agreement with some of the published experimental data. The inclusion of the higher conduction bands is expected to further improve the fit. We do not expect, however, to obtain the anisotropy measured by Pearsall et al.\textsuperscript{19} In our opinion this anisotropy is not a consequence of the band structure, but is rather caused by crystal defects or other effects not yet understood. It is found that the contribution of ballistic electrons to the impact ionization rate is negligibly small. Shockley's theory, therefore, badly underestimates the ionization rate. We have confirmed that the impact ionization rate is rather insensitive to the ionization probability above the threshold energy as long as the probability is much larger than the phonon scattering rate.

Based on the results of the simulation, a general discussion of impact ionization has been given. We find that typically electrons stay around an average energy and experience a large number of phonon scatterings. Occasionally electrons escape phonon scattering and move up to higher energy. Some reach ionization threshold after a few scattering events. This feature is seen in Fig. 16. It can be considered as a combination of Wolff's and Shockley's notion of ionizing electrons, but the distinction is rather vague. The reason for the success of Baraff's theory is that his theory also contains this feature. However, because of his formulation using distribution functions, the physical picture is not as clear as in our result (Fig. 16). Moreover, our method includes realistic scattering mechanisms and band structure.

Unlike previous theories of impact ionization, the present method can in principle be applied to any semiconductor. The method can be used for both polar and nonpolar materials. This is obvious from the successful simulation of the Gunn effect, which
contains the transition from polar optical scattering to intervalley scattering. The calculation of hole-initiated ionization rates should also be possible, although presently our understanding of hole transport is not as deep as electron transport. This is important for the understanding of the operation of photodetectors, since their performance depends on the ratio of electron- and hole-initiated ionization rates. It should be understood that the method is quite versatile in its application. A transient Monte Carlo method including the band structure may be used to investigate the orientation dependence of the avalanche response. Finally, the inclusion of the position dependence should enable us to study the effect of the "dark space." 19

ACKNOWLEDGMENTS

The authors wish to thank E. M. Kisler, R. T. Gladin, and R. F. MacFarlane for technical assistance. They are grateful to Professor G. E. Stillman, Professor B. G. Streetman, and Professor N. Holonyak, Jr., for many valuable discussions. The use of the computer facilities of the Materials Research Laboratory, University of Illinois, is also gratefully acknowledged. The work was supported by the Office of Naval Research and the Joint Services Electronics Program.

34J. Price (private communication).
drive current for a constant magnetic field and the results are plotted in Fig. 4. The 50 Hz oscillating magnetic field was supplied by a solenoid 0.295 m long and the mean field strength was 3.93 mT r.m.s. The detector output reached a maximum value of 4.77 x 10^-4 r.m.s. as the polarisation ratio increased. This corresponds to a Faraday rotation of about 0.14° r.m.s. Using the magnetic field parameters, this yields a value for the magneto-optic Verdet constant of 2.58 x 10^-6 rad A^-1 at 830 nm wavelength. This figure is in excellent agreement with the value obtained by extrapolating visible wavelength data using the reciprocal square wavelength dependence of the Verdet constant.

![Graph of r.m.s. detector output against current](image)

**Fig. 4** Graph of r.m.s. detector output against current

**Conclusion:** The polarisation properties of single-mode double-heterostructure stripe lasers make them suitable light sources for optical-fibre current measurement systems and they should be useful in any optical fibre system where a linearly polarised light source is required.

**Acknowledgment:** This work was carried out at the Central Electricity Research Laboratories and is published by permission of the Central Electricity Generating Board.

A. M. SMITH

Central Electricity Research Laboratories
Kelin Avenue
Leatherhead, Surrey KT22 7SE, England

**References**


**ORIENTATION DEPENDENCE OF BALLISTIC ELECTRON TRANSPORT AND IMPACT IONISATION**

**Indexing terms:** Charge carriers, Semiconductors

The orientation dependence of ballistic electron transport in GaAs is investigated using the pseudopotential band structure. It is shown that a single scattering event can permit electron impact-ionisation threshold energies to be reached in the (111) and (100) directions. This is in contrast to ballistic calculations, where simple thresholds do not exist in these directions.

Ballistic transport of carriers is important for the understanding of impact ionisation in semiconductors. Shockley's theory of impact ionisation considers those electrons which have escaped the scattering events and ballistically reach the threshold energy. Recently, Capasso et al. have shown that ballistic motion competes with inter-valley scattering in determining electron dynamics in GaAs. Ballistic transport can also be utilised in low-power high-speed logic devices. It is the purpose of this letter to present the results of detailed calculations which confirm that the ballistic motion of electrons in GaAs depends sensitively upon the crystallographic direction of the electric field. However, the calculations also show that one phonon-scattering event is sufficient for an electron to reach the threshold energy for impact ionisation with an electric field applied in the (111) direction, even though there is no threshold state for ballistic electron-initiated impact ionisation in this crystalline direction.

The ballistic electron behaviour is studied by solving the equations of motion:

\[
\frac{dh}{dt} = eF
\]

and

\[
\mathbf{v} = \mathbf{V} \cdot \mathbf{E}(\mathbf{k})
\]

where \( F \) is the applied electric field, \( \mathbf{v} \) is the electron wave vector, \( E \) is the electron energy and \( \mathbf{v} \) is the group velocity of the electron. The band structure \( E(\mathbf{k}) \) is calculated by employing the empirical pseudopotential method of Cohen and Bergstresser. Eqs. 1 and 2 have been solved in successive small time intervals with the initial condition \( \mathbf{k} = \mathbf{k}_0 \) at \( t = 0 \). The field \( F \) is assumed to be constant, i.e. we are interested only in cases where a few ballistic electrons cause the impact ionisation.

![Graph of r.m.s. detector output against current](image)

**Fig. 4** Variation of ballistic electron velocity with time.
chosen to be 500 kV cm. Fig. 1 shows the electron velocity \( v \) as a function of time. The orientation dependence of ballistic behaviour is obvious from this Figure. The highest peak velocity
time as measured from the conduction-band edge. The rate of increase is largest in the \( \langle 100 \rangle \) direction and smallest in the \( \langle 111 \rangle \) direction. Of course, ballistic transport must compete with the scattering processes. The dominant scattering mechanism for electron energies greater than 0.35 eV is inter-valley scattering. The momentum relaxation time for this scattering process is about \( 2 \times 10^{-14} \) s. Figs. 1 and 2 show that, even within this short timespan, the effect of orientation can be considerable. Ballistic electron transport can occur on longer time scales, but only with decreasing probability.

The orientation trend in Figs. 1 and 2 agrees with experimental results which show that, in GaAs, the electron impact ionisation rates are higher in the \( \langle 100 \rangle \) and the \( \langle 110 \rangle \) direction than in the \( \langle 111 \rangle \) direction. The distance which an electron can travel in \( 2 \times 10^{-14} \) s also reflects the same orientation dependence: 0.039 \( \mu \)m, 0.034 \( \mu \)m and 0.031 \( \mu \)m in the \( \langle 100 \rangle \), \( \langle 110 \rangle \) and \( \langle 111 \rangle \) directions, respectively, for an electric field of 500 kV/cm.

In the \( \langle 111 \rangle \) direction, the electron can never gain sufficient energy ballistically for impact ionisation. In the \( \langle 100 \rangle \) direction, the impact-ionisation threshold can be reached only if electrons tunnel in \( k \)-space to the next higher band \( \sim 0.2 \) eV above the principal conduction band. As a result, scattering events become crucial for the occurrence of impact ionisation in these directions. Electrons can be scattered to other regions of the Brillouin zone, and a single scattering event is sufficient to permit the electrons to reach threshold energy. This mechanism is illustrated in Figs. 3 and 4. An electron starts at the point and moves along the \( \langle 111 \rangle \) direction. At point A, \( \langle k \rangle \sim 0.3 \sqrt{3} \pi /a \), the energy is at the maximum for this direction, but it is still much less than the threshold energy. Subsequently, the electron can be scattered (e.g. by a phonon or impurity) to some other point in the first Brillouin zone; point B, for example. Following this scattering event, the \( \langle 111 \rangle \) component of the electron wave vector continues to increase. However, the wave vector points in a direction different from \( \langle 111 \rangle \) such that the electron can now reach a higher energy. As shown in Fig. 4, the electron can actually exceed the threshold for impact ionisation. This clearly indicates the importance of scattering processes to impact ionisation. We also note that since \( V \) is not always in the direction of the electric field for

**Fig. 2** Variation of electron energy with time as measured from the conduction band edge

**Fig. 3** \( \langle 111 \rangle \) section of the first Brillouin zone

**Fig. 4** Variation with time of electron energy for the process shown in Fig. 1
NEAR-FIELD DISTRIBUTIONS IN SELECTIVELY EXCITED ELLIPTICAL OPTICAL FIBRES

Indexing terms: Optical fibres, Wave propagation

Short (1-400 m) multimode fibres were excited by a single-mode fibre. The resulting near-field intensity distributions are generally not circularly symmetric. A calculation based on ray optics shows that slightly elliptical fibres give similar distributions. This calculation assumes a central index-profile dip.

Introduction: Recently the nature of ray propagation in elliptical fibres has been investigated by several authors. In particular, Ankiewicz has plotted diagrams depicting the paths of representative rays in elliptical fibres. In this letter, we will extend these results to profiles containing a central index dip and show that they can be verified experimentally.

Apparatus: Light from a d.h. laser operated below threshold is collimated through a half-metre length of a single-mode fibre with a core radius of 5 μm and an n.a. of 0.04. The emerging beam is then coupled to a multimode fibre, typically of core diameter 50 μm and n.a. = 0.2. The resulting near-field distribution is focused onto a 100 × 100 c.c.d. photodiode matrix and displayed on an oscilloscope.

References
2 Capasso, F., Nahory, E., and Pollak, M. A.: 'Hot electron dynamics in GaAs avalanche devices: competition between ballistic behavior and intervalley scattering', ibid., 1979, 22, pp. 977-979

Results: Figs. 1 and 2 are near-field patterns produced by a typical nearly parabolic c.d.v. fibre with a 1-2 μm central index dip and an ellipticity (defined as the ratio of the major to the minor axis) of the order of 1/10. Fig. 1 shows the near-field distribution of a 1 m fibre sample excited near the edge of its core and along one of its principal axes. Fig. 2 is produced by a 40 m length of the same fibre excited near the edge of the core and at an angle of 45° with the major axis. If we excite other
Calculation are reported showing that in multilayered heterojunction structures the effective impact ionisation rates for electrons and holes can be very different, even if they are the same in the basic bulk materials. The reason for this is that the difference in the band-edge discontinuities for electrons and holes and the lower phonon mean free path for holes in quantum well structures.

As is well known, the signal/noise ratio of an avalanche photodiode (a.p.d.) is influenced by the statistics of the gain process, and, because of feedback effects, significantly more noise is generated when both electrons and holes produce secondary carriers.

As mentioned above, the band-edge discontinuity is steplike with uniform optical phonon mean free path;  for detection at various wavelengths it is useful to use III–V compounds and ternary and quaternary alloys of these compounds in which the bandgap is only slightly smaller than the energy of the optical phonon. Unfortunately, preliminary measurements of  and  seem to indicate that in most of these materials the electron and hole impact ionisation rates are nearly equal. It is the purpose of this letter to show that two effects specific to multiheterostructure quantum layers may be useful in the construction of low noise a.p.d.s from materials in which  and  are approximately equal.

The basic physical ideas are as follows:

(i) The impact ionisation rate depends exponentially on the impact ionisation threshold and on the energy from which the electron (hole) starts to be accelerated. Therefore a step-like band structure as shown in Fig. 1, where the discontinuity in the conduction band is greater than that in the valence band, will enhance the ionisation rate for electrons. This can easily be seen by subtracting (adding) the conduction band-edge step to the ionisation threshold in the Baraff theory. A rigorous justification for this procedure can only be given for special cases, because in general the effect of the band-edge step on the ionisation rate will depend on the energy which the electron already has when it approaches the junction.

(ii) As shown by Holonyak and co-workers, the scattering rate in quantum wells is different to that in the bulk and, at low energies at least, holes are scattered more often and thus are collected more effectively in the quantum wells. An analysis of this effect is difficult because it must include the reflection and transmission through the (nonideal) heterojunction. However, inserting different mean free paths in the Baraff theory shows immediately that this effect can strongly change the  ratio if it prevails up to the energy of the impact ionisation threshold.

The following estimates are based on a structure appropriate for GaAs–AlGaAs. As layers with the material constants adjusted to give  when inserted in the Baraff theory for bulk material. A polynomial fit to the Baraff theory is used in the calculations. The values of the material constants are listed in Table I.

<p>| | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$E_t$</td>
<td>$\lambda$</td>
<td>$d$</td>
</tr>
<tr>
<td>Electron</td>
<td>2 eV</td>
<td>50 Å</td>
<td>150 Å</td>
</tr>
<tr>
<td>Hole</td>
<td>1.5 eV</td>
<td>40 Å</td>
<td>150 Å</td>
</tr>
</tbody>
</table>

When it arrives in the GaAs it 'sees' not only the smaller bandgap of the GaAs, but it also starts at an energy $\Delta E_c$ (conduction band edge step) above the GaAs band edge. To include this effect, we deduct the 'excess' energy $\Delta E_c$, from the GaAs impact ionisation threshold within a distance from the discontinuity equal to the impact ionisation mean free path. This process increases $\times$ much more than  since, when the same procedure is followed for holes, the valence band edge step $\Delta E_v$ is much smaller.

The thickness of the layers should be chosen so that after an electron impact ionises in the GaAs layer it can gain sufficient energy in this layer to get out of the well, and after the electron
enters the $\text{Al}_{x}\text{Ga}_{1-x}\text{As}$ layer with small kinetic energy, it gains the effective threshold energy $E_i(\text{GaAs}) = \Delta E_i$ before arriving at the next GaAs layer. $E_i(\text{GaAs})$ is the impact ionisation threshold for bulk GaAs. Note that the values of the layer width $x$, vary for different design parameters, i.e., doping concentration $N_\rho$, the applied voltage and the position within the structure. However, the calculated value of the thickness is always close to 300 Å for GaAs layers, and 500 Å for the $\text{Al}_{x}\text{Ga}_{1-x}\text{As}$ layer.

The above procedure gives immediately the $z/\beta$ ratio at a particular location in the layers. The value of $z/\beta$ relevant to the multiplication factor in an a.p.d. is given by the spatial average over the whole structure. Our results for the average $z/\beta$ ratio are shown in Fig. 2. As can be seen the enhancement of the $z/\beta$ ratio is substantial especially for low values of the donor density $N_\rho$. The multiplication factor is in an interesting range (i.e., of the order of 10 or larger) only for the two highest doping concentrations shown in Fig. 2. The reasons for this are outlined below.

The second effect which enhances $z/\beta$, the higher phonon scattering rate of holes in the heterojunction structures, has not been included in the results of Fig. 2. It is clear that this effect once more increases $z/\beta$. In fact the mean free path for phonon scattering enters more sensitively in the impact ionisation rate than the ionisation threshold. The amount of the reduction of mean free path is not known exactly, as the results of Holonyak and co-workers apply only for electrons with rather low energy. We therefore have changed the hole mean free path rather arbitrarily from 40 Å to 30 Å in the GaAs quantum wells to demonstrate the effect. The result for the average $z/\beta$ ratio is shown in Fig. 3, once more against the number of wells.

From the above discussion it is clear that the $z/\beta$ ratio depends sensitively on the structure and doping concentration. This is due to the fact that $z$ is considerably larger than $\beta$ only for electric fields $E < 10^4$ V/cm. Therefore, if we choose to increase the multiplication factor, we automatically reduce the $z/\beta$ ratio. Nevertheless, the above analysis shows that even for multiplication factors above 10 the $z/\beta$ ratio can be substantially enhanced in quantum well structures, especially because of the second enhancement effect, the reduction of the phonon mean free path. Finally we would like to note that fluctuating fields associated with compositional disorder in ternaries and quaternaries have an effect similar to the band-edge discontinuity at the heterojunction and can increase (decrease) the $z/\beta$ ratio. Work is in progress on these effects and will be reported later.

Acknowledgments: The authors wish to thank E. M. Kesler, S. B. Marshall, R. T. Gladin and R. F. MacFarlane for technical assistance. The work has been supported by NSF Grants DMR-79-09991 and DMR-23999 and Navy contract N00019-79-C-0768.

R. CHIN*
N. HOLONYAK, JUN.
G. E. STILLMAN
Department of Electrical Engineering
& Materials Research Laboratory
University of Illinois at Urbana-Champaign
Urbana, Ill. 61801, USA

J. Y. TANG
K. HESS
Department of Electrical Engineering
& Coordinated Science Laboratory
University of Illinois at Urbana-Champaign
Urbana, Ill. 61801, USA

* Now at Rockwell International, Thousand Oaks, California, USA

References

0013-5194/80/120467-03 $1.50/0
Phonon contribution to double-heterojunction laser operation

N. Holonyak, Jr., B. A. Voják, and W. D. Ladig
Department of Electrical Engineering and Materials Research Laboratory, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801

K. Hess
Department of Electrical Engineering and Coordinated Science Laboratory, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801

J. J. Coleman and P. D. Dapkus
Rockwell International Electronics Research Center, Anaheim, California 92803

(Received 21 February 1980; accepted for publication 12 May 1980)

Laser data (77 and 300 K) are presented on two photopumped undoped metalorganic chemically vapor-deposited Al_{x}Ga_{1-x}As-GaAs heterostructures with active regions consisting of: (i) a thick GaAs layer ($L_{1} \approx 1500$ Å) coupled to an auxiliary quantum-well array of seven small $L_{2} \approx 50$ Å coupled GaAs layers, and (ii) a comparison single thick GaAs layer ($L_{1} \approx 600$ Å) in the form of a conventional double heterostructure (DH). Because of the strengthening of phonon-assisted recombination with temperature, laser operation of the bulk ($L_{1} \approx 500$ Å) GaAs layers is shifted from $\hbar \omega - E_{r}$ at 77 K to $\hbar \omega < E_{r}$ at room temperature. This behavior of the bulk DH GaAs layers agrees with that of the reference recombination radiation observed from the auxiliary quantum-well array (wafer # 1), which recent work indicates is phonon assisted.

PACS numbers: 42.55.Px, 78.55.Ds, 81.15.Gh, 85.60.Jb

Recent work has shown that phonon involvement in the laser operation of quantum-well heterostructure (QWH) lasers is readily observed\(^1\) and, in fact, should be expected.\(^2\) It is even possible to induce phonon-sideband laser operation of a single larger quantum well with a phonon generating array (a phonon resonator) of smaller quantum wells.\(^3\) In contrast, phonon-sideband laser operation of a standard double heterostructure (DH), i.e., a DH of active-region thickness $L_{1} \geq 500$ Å and here assumed (as is common) lightly doped or undoped ($< 10^{17}$/cm\(^3\) ), has not been identified even though laser operation of a undoped DH GaAs active region is commonly observed 30–35 meV below the band gap $E_{g}$.\(^4\) It is not uncommon in such a case to propose some sort of model involving unexplained impurities,\(^5\) which, if acceptors, would have to exceed a density of $10^{17}$/cm\(^3\) to have much validity.\(^10\) In this letter we describe experiments indicating that for standard DH lasers, with undoped active regions ($n_{d} = n_{i} \lesssim 10^{15}$/cm\(^3\) ), it is also phonon participation that accounts for the laser operation at reduced energy ($\hbar \omega < E_{r}$). The effect of phonons is observed by coupling a quantum-well phonon generating and reflecting array of seven coupled 50-Å GaAs wells to a bulk DH GaAs active region ($L_{1} = 1500$ Å),\(^6\) and by comparing the shift with temperature of the recombination radiation of the bulk GaAs and the phonon-sideband marker radiation of the small-well array. At 300 K the recombination radiation is shifted by $-\hbar \omega_{LO}$.

The two Al\(_{x}\)Ga\(_{1-x}\)As-GaAs heterostructures constructed for this work are grown by metalorganic chemical vapor deposition (MOCVD).\(^1\)–\(^3\) A GaAs buffer layer is grown first on a [100] GaAs substrate and is followed by a $\sim 1$-µm-thick Al\(_{x}\)Ga\(_{1-x}\)As ($x \approx 0.36$) confining layer, then the active region, and finally another confining layer ($x \approx 0.36$) of thickness $\sim 0.3$ µm. The active region of the first wafer consists of a 1500-Å (bulk) GaAs layer coupled to an array of seven small GaAs quantum wells ($L_{2} \approx 50$ Å) which are in turn coupled by $\sim 50$-Å Al\(_{x}\)Ga\(_{1-x}\)As ($x \approx 0.32$) barrier layers. The second wafer is similar to the first except for the active region, which is a single GaAs layer of thickness $L_{1} \approx 600$ Å. To eliminate the possibility of band-to-impurity laser transitions, all layers in the wafers are...

**Fig. 1.** Pulsed laser operation (4.8 × 10\(^3\) W/cm\(^2\), 77 K) of a photopumped undoped ($n_{d} = n_{i} \lesssim 10^{15}$/cm\(^3\) ) MO-CVD Al\(_{x}\)Ga\(_{1-x}\)As-GaAs multiple-quantum-well heterostructure. The sample is 23 × 390 µm\(^2\) in size and has an active region (confined between $-1$ and $-0.3$ µm x $-0.36$ Al\(_{x}\)Ga\(_{1-x}\)As layers) consisting of one bulk $L_{1} \approx 1500$-Å GaAs layer and seven thin $L_{2} \approx 50$-Å GaAs layers, all coupled by 50-Å-thick Al\(_{x}\)Ga\(_{1-x}\)As ($x \approx 0.32$) barriers. At low temperature laser operation is observed on and slightly above the GaAs band edge (band-to-band transitions, $\hbar \omega - E_{r}$). A spontaneous emission reference peak is also observed ($\sim 10$ inset) near and on the broadened $n = 1$ electron-to-heavy-hole transitions of the auxiliary quantum-well array (seven coupled 50-Å GaAs layers).
the "LO" markers. Electron-to-heavy-hole and down peak diamond window and undoped quantum-well heterostructure cited. Thus, if the emission of the quantum-well temperature sensitive nor in the present case very heavily phonon ray. The quantum-well transitions to-light-hole transitions of the auxiliary quantum-well array, which is located very close to the broadened wavelength a small emission bump, which serves as a reference emission bump and is peaked (a, spontaneous emission, 10³ W/cm², 300 K) well above the band edge, or in the region of the n = 3 or 4 electron-to-heavy-hole transitions if they could be identified. At high excitation levels, as here, band filling easily reaches into this region. Laser operation at higher excitation (b, 4.7 x 10⁴ W/cm²) occurs about one phonon below "transitional" n = 3 (here inserted simply as a reference), which is well below E₄. At 77 K the laser operation (c, 2.5 x 10⁴ W/cm², i.e., comparable excitation level) occurs distinctly on the band edge, which indicates that impurities are not important in the recombination process nor carrier-induced band-gap shrinkage. It is interesting to note that the physical structure of a DH laser is important in respect to the phonon contribution to its operation. First, the major discontinuity in energy gap from the AlGaAs, As confining layers to the GaAs active region requires many LO phonons to be emitted in the process of carrier injection ("hot" carriers) and carrier thermalization. Also, the LO phonons are expected, because of grown undoped (n_d = n_c ≤ 10¹⁵/cm³). The GaAs substrate is removed by polishing and selective etching; the remaining ~1.4-μm-thick wafer is cleaved into samples of dimensions ~50 x ~150 μm (average) which are heat sunk and then photoexcited with an Ar⁺ laser (λ ~ 5145 Å) focused to a circular spot with a diameter comparable to the sample width.

The 77-K emission spectrum of a rectangular sample cleaved from the first wafer is shown in Fig. 1. Two features are apparent: (i) Laser operation occurs on or somewhat above (high excitation, 4.8 x 10⁴ W/cm²) the band edge E₄ of the bulk GaAs layer (Lₐ ~ 1500 Å). (ii) At much shorter wavelength a small emission bump, which serves as a reference, is located very close to the broadened n = 1 electron-to-heavy-hole transitions (dark marker) of the seven coupled 50-Å GaAs quantum wells. The two "LO" markers show where this bump would be located if, as hot carriers thermalize, much phonon generation occurred in the coupled 50-Å quantum wells, as is indeed the case when this section is a bigger fraction of the active region (> 0.5).

The behavior of this material (wafer #1) changes radically at 300 K (Fig. 2). The laser emission shifts to well below the band edge, E₄ ~ E₄LO < E₄. This agrees with the shift of the reference emission bump one phonon, E₄LO, below the n = 1 electron-to-heavy-hole or the n' = 1' electron-to-light-hole transitions of the auxiliary quantum-well array. The quantum-well transitions are expected to be phonon assisted but, as discussed below, are not very temperature sensitive nor in the present case very heavily excited. Thus, if the emission of the quantum-well array shifts with temperature, the emission of the bulk GaAs layer is certain to shift, provided phonon-assisted recombination governs its behavior.

The behavior of the second wafer, which is near the boundary in size between bulk and quantum-well dimensions, is shown in Fig. 3. For the 600-Å active region, and no auxiliary quantum-well array, the emission is free of the reference emission bump and is peaked (a, spontaneous emission, 10³ W/cm², 300 K) well above the band edge, or in the region of the n = 3 or 4 electron-to-heavy-hole transitions if they could be identified. At high excitation levels, as here, band filling easily reaches into this region. Laser operation at higher excitation (b, 4.7 x 10⁴ W/cm²) occurs about one phonon below "transitional" n = 3 (here inserted simply as a reference), which is well below E₄. At 77 K the laser operation (c, 2.5 x 10⁴ W/cm², i.e., comparable excitation level) occurs distinctly on the band edge, which indicates that impurities are not important in the recombination process nor carrier-induced band-gap shrinkage.

It is interesting to note that the physical structure of a DH laser is important in respect to the phonon contribution to its operation. First, the major discontinuity in energy gap from the AlGaAs, As confining layers to the GaAs active region requires many LO phonons to be emitted in the process of carrier injection ("hot" carriers) and carrier thermalization. Also, the LO phonons are expected, because of grown undoped (n_d = n_c ≤ 10¹⁵/cm³). The GaAs substrate is removed by polishing and selective etching; the remaining ~1.4-μm-thick wafer is cleaved into samples of dimensions ~50 x ~150 μm (average) which are heat sunk and then photoexcited with an Ar⁺ laser (λ ~ 5145 Å) focused to a circular spot with a diameter comparable to the sample width.

The 77-K emission spectrum of a rectangular sample cleaved from the first wafer is shown in Fig. 1. Two features are apparent: (i) Laser operation occurs on or somewhat above (high excitation, 4.8 x 10⁴ W/cm²) the band edge E₄ of the bulk GaAs layer (Lₐ ~ 1500 Å). (ii) At much shorter wavelength a small emission bump, which serves as a reference, is located very close to the broadened n = 1 electron-to-heavy-hole transitions (dark marker) of the seven coupled 50-Å GaAs quantum wells. The two "LO" markers show where this bump would be located if, as hot carriers thermalize, much phonon generation occurred in the coupled 50-Å quantum wells, as is indeed the case when this section is a bigger fraction of the active region (> 0.5).

The behavior of this material (wafer #1) changes radically at 300 K (Fig. 2). The laser emission shifts to well below the band edge, E₄ ~ E₄LO < E₄. This agrees with the shift of the reference emission bump one phonon, E₄LO, below the n = 1 electron-to-heavy-hole or the n' = 1' electron-to-light-hole transitions of the auxiliary quantum-well array. The quantum-well transitions are expected to be phonon assisted but, as discussed below, are not very temperature sensitive nor in the present case very heavily excited. Thus, if the emission of the quantum-well array shifts with temperature, the emission of the bulk GaAs layer is certain to shift, provided phonon-assisted recombination governs its behavior.

The behavior of the second wafer, which is near the boundary in size between bulk and quantum-well dimensions, is shown in Fig. 3. For the 600-Å active region, and no auxiliary quantum-well array, the emission is free of the reference emission bump and is peaked (a, spontaneous emission, 10³ W/cm², 300 K) well above the band edge, or in the region of the n = 3 or 4 electron-to-heavy-hole transitions if they could be identified. At high excitation levels, as here, band filling easily reaches into this region. Laser operation at higher excitation (b, 4.7 x 10⁴ W/cm²) occurs about one phonon below "transitional" n = 3 (here inserted simply as a reference), which is well below E₄. At 77 K the laser operation (c, 2.5 x 10⁴ W/cm², i.e., comparable excitation level) occurs distinctly on the band edge, which indicates that impurities are not important in the recombination process nor carrier-induced band-gap shrinkage.

It is interesting to note that the physical structure of a DH laser is important in respect to the phonon contribution to its operation. First, the major discontinuity in energy gap from the AlGaAs, As confining layers to the GaAs active region requires many LO phonons to be emitted in the process of carrier injection ("hot" carriers) and carrier thermalization. Also, the LO phonons are expected, because of grown undoped (n_d = n_c ≤ 10¹⁵/cm³). The GaAs substrate is removed by polishing and selective etching; the remaining ~1.4-μm-thick wafer is cleaved into samples of dimensions ~50 x ~150 μm (average) which are heat sunk and then photoexcited with an Ar⁺ laser (λ ~ 5145 Å) focused to a circular spot with a diameter comparable to the sample width.

The 77-K emission spectrum of a rectangular sample cleaved from the first wafer is shown in Fig. 1. Two features are apparent: (i) Laser operation occurs on or somewhat above (high excitation, 4.8 x 10⁴ W/cm²) the band edge E₄ of the bulk GaAs layer (Lₐ ~ 1500 Å). (ii) At much shorter wavelength a small emission bump, which serves as a reference, is located very close to the broadened n = 1 electron-to-heavy-hole transitions (dark marker) of the seven coupled 50-Å GaAs quantum wells. The two "LO" markers show where this bump would be located if, as hot carriers thermalize, much phonon generation occurred in the coupled 50-Å quantum wells, as is indeed the case when this section is a bigger fraction of the active region (> 0.5).

The behavior of this material (wafer #1) changes radically at 300 K (Fig. 2). The laser emission shifts to well below the band edge, E₄ ~ E₄LO < E₄. This agrees with the shift of the reference emission bump one phonon, E₄LO, below the n = 1 electron-to-heavy-hole or the n' = 1' electron-to-light-hole transitions of the auxiliary quantum-well array. The quantum-well transitions are expected to be phonon assisted but, as discussed below, are not very temperature sensitive nor in the present case very heavily excited. Thus, if the emission of the quantum-well array shifts with temperature, the emission of the bulk GaAs layer is certain to shift, provided phonon-assisted recombination governs its behavior.
the AlGaAs-GaAs interfaces, to be restricted to some extent to the volume of the active region.\(^9\) That the phonons are generated in such large numbers and are partially confined to such a small volume increases the probability of an electron-LO-phonon interaction and phonon assistance in recombination. Thus large-dimension GaAs (\(>1 \mu m\)), not to mention the case without confining heterostructures, when photoexcited a few \(kT\) within the energy gap has no basis to operate as a laser on an LO-phonon sideband.\(^{14}\) In fact, the results of Ref. 14 offer further data in support of the mechanism elucidated here.

As mentioned above, in a "two-dimensional" well \((L \leq 200 \text{ Å})\) the phonon emission process is expected to depend only weakly on temperature. There are two reasons for this: (i) The phonon occupation number \(N_\text{q}\) is expected to be at least \(10^7\) higher than the thermal equilibrium value for certain ranges of the wave vector \(q\) even at 300 K. (ii) Two-dimensional screening of the phonon emission process is less significant than the screening in three dimensions since the screening constant has a limiting value of \(2/a_0\),\(^{15}\) where \(a_0\) is the effective Bohr radius and is independent of temperature.

In a three-dimensional (bulk) region, on the other hand, the perturbation of \(N_\text{q}\) is estimated to be weaker, and the thermal occupation adds significantly to any "stimulated term," which is proportional to \(N_\text{q} = N_\text{q}^{\text{th}} + N_\text{q}^{\text{me}}\) where \(N_\text{q}^{\text{th}}\) is the thermal occupation and \(N_\text{q}^{\text{me}}\) is the additionally generated phonon occupation number. In addition, the phonon emission probability in three dimensions is large only for very small values of \(|q|\).\(^{16}\) Therefore screening of the electron-phonon interaction is already of high importance at rather low carrier concentrations. Also, the classical screening length exhibits a significant temperature dependence. In any case, temperature is expected and is observed to play a major role. It is difficult, however, to calculate explicit expressions for the above effects because the energy distribution of the carriers is not known.

In summary, the data and arguments above indicate that phonon-assisted recombination (300 K) is mainly responsible for lowering the emission energy of a DH laser (lightly doped or undoped active region) to the range \(\hbar \omega < E_g\). This conclusion is consistent with the high excitation level \((\sim 10^4 \text{ A/cm}^2)\) typical of DH laser operation, which provides a basis for large-phonon generation.

The authors are grateful to Yuri S. Moroz, R. T. Gladin, B. L. Marshall, and B. L. Payne (Urbana) for technical assistance, and to G. E. Stillman for helpful discussions. The work of the Illinois group has been supported by NSF Grants DMR 79-09991 and DMR 77-23999 and Navy Contract N00014-79-C-0768; the work of the Rockwell group has been partially supported by the Office of Naval Research, Contract N00014-78-C-0711.

---

**Ultrasensitive detection of aromatic hydrocarbons by two-photon photoionization**

Charles Klimcak and John Wessel

Ivan A. Getting Laboratories, The Aerospace Corporation, Los Angeles, California 90009

(Received 17 March 1980; accepted for publication 5 May 1980)

An optimized multiphoton photoionization detection system has been applied to monitor aromatic-hydrocarbon vapor density as a function of temperature. The density curves established for naphthalene by this procedure permit estimation of a detection limit of \(5 \times 10^4\) molecules/cm\(^3\) in a nitrogen buffer gas. With slight modification this method would be capable of single-molecule detection limits.

PACS numbers: 33.80.Kn, 06.70.Dn, 82.80.Di, 64.70.Hz

Recently several research groups have achieved detection limits in the single-atom regime using photoionization- and fluorescence-based techniques.\(^1\text{1}-\text{15}\) Attainment of molecular detection at densities approaching this limit is of consid-
Phonon contribution to metalorganic chemical vapor deposited Al$_x$Ga$_{1-x}$As-GaAs quantum-well heterostructure laser operation

B. A. Vojak, N. Holonyak, Jr., and W. D. Laidig
Department of Electrical Engineering and Materials Research Laboratory. University of Illinois at Urbana-Champaign. Urbana, Illinois 61801

K. Hess
Department of Electrical Engineering and Coordinated Science Laboratory. University of Illinois at Urbana-Champaign. Urbana, Illinois 61801

J. J. Coleman and P. D. Dapkus
Rockwell International. Electronics Research Center. Anaheim, California 92803

(Received 16 July 1980; accepted for publication 29 October 1980)

A series of experiments have been conducted to determine the extent of longitudinal optical (LO) phonon contribution to quantum-well-heterostructure (QWH) laser operation. Extensive data are presented on metalorganic chemical vapor deposited (MO-CVD) Al$_x$Ga$_{1-x}$As-GaAs QWH's with active regions consisting of larger quantum wells, or in some cases bulk layers ($L_z > 500$ Å), coupled to phonon-generating and -reflecting arrays of coupled smaller quantum wells. Because of the electronic and vibrational coupling of the single larger layer to the array, the spontaneous emission and laser emission from these structures differ from that of QWH's containing either a single well or a multilayer of uniform well thickness. In fact, phonon sideband laser operation of the larger GaAs layer can be induced at $\hbar \omega = E_g - \hbar \omega_{LO}$ (undoped layers, $n_s - n_\pi < 10^{15}$ cm$^{-3}$). An increase in either the thermal or nonthermal phonon occupation number is shown to cause phonon sideband laser operation in a QWH. A guide to the design of the multilayer array also is presented.

PACS numbers: 78.50.Ge, 78.45.+h, 63.20.-e, 81.15.Gh

I. INTRODUCTION

Until quite recently, the design of III-V semiconductor lasers has involved the optimization of carrier, current, and electromagnetic field confinement in some form of stripe-configuration double-heterostructure laser. As the carriers are better confined, however, so also to some extent are the longitudinal optical (LO) phonons that are emitted during the process of carrier energy relaxation from the wider-energy-gap confining layers (injecting layers) to the narrower-gaps active region. The role that phonons might play in double-heterojunction (DH) and quantum-well-heterostructure (QWH) lasers has been poorly understood in spite of the fact that large phonon densities are likely to exist in the active region at threshold, which is typically high ($J - 10^7$ A/cm$^2$). For example, in an Al$_x$Ga$_{1-x}$As-GaAs ($x = 0.4, T = 300$ K) DH laser approximately $[E_v(AlGaAs) - E_v(GaAs)]/\hbar \omega_{LO} = (1.923-1.424)/0.036 \approx 55$ LO phonons are emitted for each electron-hole pair injected into the active region. That LO phonons do modify laser action has been shown in the phonon-sideband operation of AlGaAs-GaAs,\textsuperscript{1,2} InGaPAs-InP,\textsuperscript{3,4} and InGaPAs-GaAsP,\textsuperscript{5} quantum-well heterostructures. All of these are III-V semiconductor compounds in which, unlike II-VI compounds, phonon participation in laser operation has not previously been identified. This has been more or less expected because the electron-LO phonon coupling is inherently relatively weak in comparison with II-VI compounds.

The relevant recombination and LO phonon scattering processes for undoped GaAs in the bulk and quantum-well cases are illustrated in the density of states versus energy diagram of Fig. 1. As electronic carriers are confined to a thin-lower-energy-gap semiconductor layer between two wider-gap layers, the single-particle energy spectrum takes on a particle-in-a-box character in the dimension in which

![Density of states diagram](image-url)
the layer is constricted (e.g., for GaAs $L_x < 500 \, \text{Å}$), and results in a number of quasi-two-dimensional subbands each of which has a constant density of states. The cumulative densities of states for electrons and for light and heavy holes in the quantum-well regime is steplike as shown in Fig. 1, with each step occurring at the energy of the one-dimensional confined-carrier energy. In the bulk limit, the usual parabolic density of states exists (dashed). The curved arrows on the conduction-band densities of states represent LO-phonon with all of the wells coupled.

Confined-carrier energy. In the bulk limit, the usual parabolically shaped density of states for electrons and for heavy and light holes in Si differs in a number of quasi-two-dimensional subbands each of which has a constant density of states. The cumulative density of states is shown (dashed). The curved arrows illustrate the various low-energy confined-carrier transitions. Also shown is the light- to heavy-hole relaxation.

The form of the density of states is fundamental to the process of LO-phonon emission and absorption in polar optical scattering and is so important that, in the two-dimensional limit, the basic electron-LO-phonon interaction is actually slightly enhanced over the bulk case, making stimulated phonon emission more of a possibility. Because of this, the nonthermal LO-phonon occupation number is expected to be greatly increased in QWH lasers. These phonons, however, are extremely difficult to detect. Earlier work indicates that multiple thin-layer ($L_x \leq 80 \, \text{Å}$) structures, in contrast to single ($L_x \leq 500 \, \text{Å}$) quantum wells, are very efficient in carrier collection and thermalization and operate readily on LO-phonon sidebands. A valid verification of the role of LO phonons in a QWH is, therefore, the artificial inducing of phonon-sideband laser operation in a larger quantum well ($L_x \sim 200-500 \, \text{Å}$) or bulk layer by a phonon-generating and reflecting array of small ($L_x \sim 50-80 \, \text{Å}$) quantum wells. Also, the identification of phonon-sideband laser operation of a thicker layer ($L_x \geq 200 \, \text{Å}$) is easier because of the advantage that the lowest-energy confined-carrier transitions converge to $E_g$ as $L_x$ increases; the uncertainty in determining $L_x$ and the confined-carrier transitions is thus decreased.

The purpose of the present work is to determine the extent to which LO phonons affect the laser operation ($77-300 \, \text{K}$) of both QWH and DH Al$_x$Ga$_{1-x}$As-GaAs semiconductor lasers. Phonons generated in a thin multiple QWH array are used to induce phonon-sideband emission in a larger, coupled, “phonon-detector” GaAs layer. The extensive data presented on QWH’s of various well thicknesses show that Al$_x$Ga$_{1-x}$As-GaAs heterostructure lasers can be designed which take advantage of the LO phonons that are inherently generated in these structures.

II. CRYSTAL PREPARATION AND EXCITATION

The Al$_x$Ga$_{1-x}$As-GaAs samples of interest here are grown by metalorganic chemical vapor deposition (MOCVD), which has been described extensively elsewhere. The wafers, grown at 750 °C on [100] GaAs substrates at a calibrated growth rate of ~0.25 μm/min (or slower), consist of a ~1-μm-thick GaAs buffer layer to provide a good crystallographic surface for the succeeding layers, followed by a ~1-μm Al$_x$Ga$_{1-x}$As ($x \sim 0.36$) confining layer, then the QWH active region, and finally a second ~0.3-μm Al$_x$Ga$_{1-x}$As ($x \sim 0.36$) confining layer. All layers are undoped ($n_+ - n_- < 10^8 \, \text{cm}^{-3}$).

Six different QWH active regions composed of thin-layer phonon-generating arrays coupled to larger GaAs quantum wells ($L_x \leq 500 \, \text{Å}$) or standard DH active layers ($500 \, \text{Å} \leq L_x \leq 2000 \, \text{Å}$) are employed. They are (i) a single $L_x \sim 200$-Å GaAs well and seven $L_x \sim 50$-Å GaAs wells with all of the wells coupled by seven ~50-Å-thick Al$_x$Ga$_{1-x}$As ($x \sim 0.32$) barriers [structure denoted as (1)–(7) 200–50 Å]; (ii) a structure identical to (i) with the exception that the thicker GaAs layer is changed to $L_x \sim 500$ [(1)–(7) 500–50 Å]; (iii) a structure identical to (i) with the exception that the larger GaAs well is increased in size to $L_x \sim 1500$ [(1)–(7) 1500–50 Å]; (iv) a structure similar to (i) with $L_x \sim 160, L_x \sim 80$ Å and with ~80-Å-thick Al$_x$Ga$_{1-x}$As ($x \sim 0.32$) coupling barriers [(1)–(7) 160–80 Å]; (v) a phonon-generating array of seven $L_x \sim 50$-Å GaAs wells on either side of an $L_x \sim 500$-Å GaAs layer all of which are coupled by fourteen ~50-Å-thick GaAs wells.

![FIG. 2. Scanning-electron microscope photograph of a multiple-quantum-well heterostructure grown by MOCVD with an active region consisting of seven 50-Å GaAs wells and one 500-Å GaAs well coupled by seven 50-Å Al$_x$Ga$_{1-x}$As ($x \sim 0.32$) barriers. The cleaved and stained cross section shows the 500-Å GaAs layer (right-hand arrows); the left-hand arrows indicate the array of seven 50-Å layers, which cannot be individually resolved. Photograph b shows a shallow-angle beveled and stained cross section of the same QWH. The shallow-angle bevel and stain cause the layers to appear enlarged (by a factor of 93 for this cross section), allowing the array of seven 50-Å wells and seven 50-Å barriers to be resolved (left-hand arrows).](image)
AlGaAs wells coupled via [I-1-7] 50-500-50 Å, and
(iii) two $L_{31}$ ~ 120-Å GaAs wells with one located on either side
of an array of six $L_{11}$ ~ 80-Å GaAs wells with all of the
GaAs layers coupled by seven ~ 80-Å-thick AlGaAs wells with
an $x$ ~ 0.32 barrier layers [I-1-6-1] 80-120 Å. In addition to
the undoped wafers described above, four "degenerate" cases with
the substrate side down to a thickness of ~ 50 μm and then
selectively etching off the GaAs substrate and buffer layer. The resulting thin (~ 1.4-μm-thick) wafer is then cleaved into rectangular samples ~ 10-100 μm wide by
~ 100-300 μm long which are imbedded into In under a
sapphire window for 77 K operation or into annealed Cu
under diamond for 300 K operation. Typically, a circular
spot of Ar laser light comparable in diameter to the sample
width is used to excite electron-hole pairs in the
AlGaAs, as confining layers. Since $\alpha L_{31} \ll 1$, most of the
carriers are generated in the confining layers. The carriers
diffuse to the active region where they thermalize by emitting
LO phonons and then recombine. The one ($5 + 6$) 80-Å
structure that is grown sandwiched between $n$- and $p$-type
confining layers has been both fabricated into simple stripe-
geometry laser diodes and has been processed into a photolu-
mescence sample by selectively etching off the GaAs
strate and contact layers.

III. EXPERIMENTAL DATA

The emission spectra of a large quantum well ($L_{31}$
≥ 200 Å) coupled to an array of small wells ($L_{11}$ ≤ 80 Å) dif-

![FIG. 3. Pulsed photoluminescence spectra (77 K) of a sample (535 × 438 μm²)
cleaved from a heterostructure similar to that shown in Fig. 2 but with a
200-Å GaAs layer in place of the 500-Å layer. A one-dimensional model
of the conduction band and the allowed electron energy levels is indicated by
the inset. The heavy and light bars on the horizontal axis mark the transition
energies for electrons to recombine with heavy holes ($e\rightarrow h$, $n$ confined-
particle transitions) or with light holes ($e\rightarrow l$, $n$ confined-particle
transitions) respectively. The spontaneous spectrum shows the emission just
below lasing threshold [1, 2 × 10⁶ W/cm²]. At slightly higher excitation
power [3, 7.0 × 10⁶ W/cm²] the main laser mode occurs on the $n = 1$
transition with the simultaneous occurrence of a small spectral bump at
energy $h\nu_{0}$ below the $n = 1$ transition. At higher power [4, 10⁶ W/cm²]
the small bump develops into a well-defined laser mode.](https://example.com/figure3)
fer markedly from those of a single large well \( L \geq 200 \text{ Å} \), or from a degenerate multilayer structure \( L \leq 80 \text{ Å} \) in which all the quantum wells are the same thickness. The proximity \( L \leq 80 \text{ Å} \) of a larger well to an array (see inset of Fig. 3) is very important in the electronic and vibrational coupling of the two systems. Both electrons, which have a significant tunneling probability for an \(-80\text{-Å-thick} \sim 400\text{-meV} \) rectangular barrier, and LO phonons, with a 100-500-Å mean free path, are likely to be shared in the whole system and affect the recombination and inelastic scattering processes. For example, LO phonons generated in the small-well arrays of these heterostructures influence the recombination in the larger layers.

Typical emission spectra (77 K) of a photopumped, rectangular sample from the (1-7) 200-50-Å wafer (i) are shown in Fig. 3. The form of the conduction-band edge in the vicinity of the active region is illustrated in the inset. The horizontal lines indicate the electron eigenenergies of this one-dimensional potential. These lines are sketched to correspond to the spatial extent of the wavefunctions. The numbers 1-6 on the left side of the lines and the 1 and 2 on the right side denote those states of the system which arise because of the \( L_{14} \sim 200\text{-Å-thick} \) well and the \( L_{24} \sim 50\text{-Å} \) multilayer, respectively. While this numbering scheme is not strictly correct for the complete coupled quantum system, it is very useful since some eigenfunctions are more localized in the \( L_{14} \sim 200\text{-Å} \) well and others are more localized in the \( L_{24} \sim 50\text{-Å} \) multilayer. Note that this localization should not restrict the motion of the electrons since the very-small-layer dimensions easily allow electron tunneling between the multilayer and the larger GaAs layer.

The (1-7) 200-50-Å sample, when pulse excited \( (6.2 \times 10^3 \text{ W/cm}^2) \) partially across its width, exhibits the high-level spontaneous emission spectrum, Fig. 3(a). Spontaneous emission peaks are observed at slightly lower energies than the first electron-to-heavy-hole \( n = 1 \) confined-carrier transitions of both the multilayer array and the larger quantum well. With an increase in pump power to \( 7 \times 10^4 \text{ W/cm}^2 \), Fig. 3(b), a laser mode appears abruptly near the first electron-to-light-hole \( n' = 1 \) transition of the \( L_{14} \sim 200\text{-Å} \) GaAs well, and simultaneously a small bump emerges \( \sim 0 \text{ at } 7 \times 10^4 \text{ W/cm}^2 \) this bump also lasse although it is still much lower in intensity than the higher-energy confined-carrier stimulated emission. The location in energy and the unique manner of turn-on of the bump with the laser line are interpreted as evidence for stimulated photon emission.

The emission spectrum (77 K) of a second sample from the (1-7) 200-50-Å wafer is shown in Fig. 4. At low-level cw excitation [curve (a), \( 250 \text{ W/cm}^2 \)] the spontaneous emission peaks at very nearly the same energies as the sample of Fig. 3. For pulsed excitation, however, laser operation is observed [curve (b), \( 5 \times 10^4 \text{ W/cm}^2 \)] both on a phonon sideband of the lowest-confined-carrier transitions and also near the \( n = 2 \) transition of the \( L_{12} \sim 200\text{-Å-} \) well. Note that with this sample and excitation geometry the phonon-sideband laser modes can be made to dominate the emission spectrum as opposed to the relatively weak modes at that energy shown in Fig. 3. That this effect is primarily due to the excitation geometry can be seen by comparing the spectrum of Fig. 4 with that of Fig. 3(b) of Ref. 8. Both spectra are from the same cleaved sample \( (28 \times 244 \text{ µm}^2) \) and are excited to the same level \( (5 \times 10^3 \text{ W/cm}^2) \). However, the pump beam is at a slightly different location of the sample in the two cases: this results in the relative emission intensities of the phonon sideband and the higher-energy laser modes to be different.

As mentioned earlier, this type of emission spectrum, i.e., with stimulated emission occurring \( \sim n_0 \) lower in energy than the lowest-confined-carrier transition, is not similar to that of a single \( \sim 200\text{-Å-thick} \) well. Depending on sample and pump beam geometry and also the excitation power, laser action has occurred over a very broad energy range in a single \( L \sim 200\text{-Å-} \) QWH (see Fig. 10 of Ref. 9). However, it has not been observed as low in energy as \( n_0 \) below the lowest \( n = 1 \), \( n' = 1 \) transitions of both the multilayer array and the larger GaAs well. Smaller GaAs layers to a single \( L \sim 200\text{-Å} \) GaAs well as \( 7 \times 10^4 \text{ W/cm}^2 \) walk, the carrier collection, thermalization, and bandfilling problems are drastically reduced. Most of the carriers are collected by and scatter to lower energy in the multilayer portion (64% of the GaAs

![Graph](https://example.com/image.png)
A further interesting feature of the (1–7) 200-50-Å QWH is the presence of emission and laser modes in the range between the lowest-energy confined-carrier transitions of the system and the phonon sidebands. This is demonstrated clearly in the 77 K photoluminescence spectra of Fig. 6. As with the spontaneous emission data of Figs. 3, curve (a), and 4, curve (a), the CW emission at low level [Fig. 6, emission (a)] exhibits a shoulder approximately 20 meV below the n = 1 transition, corresponding to the expected binding energy of a two-dimensional exciton in GaAs. At higher power [Fig. 6, emission (b)] a well-defined group of laser modes labeled A, B, and C, 20 meV below the n = 1 marker) appears as well as laser operation on a phonon-sideband laser modes observed in the data from the same wafer described in Fig. 3. Besides the low-level (250 W/cm²) spontaneous-peak laser modes observed in the data from the same wafer described in Fig. 3, this results in two-dimensional-exciton binding energies of ~20 meV for electron-heavy-hole exciton and ~13 meV for the electron-light-hole exciton. The 4× increase over the three-dimensional case is expected in the limit of two-dimensional confinement and will be reduced to 1× as the layer thickness is increased to the bulk limit. For layer thicknesses less than the bulk-exciton diameter (~240 Å e-h, ~340 Å e-h), the factor of 4× continues to agree well with photoluminescence data; this is in contrast to earlier absorption measurements (on crystals grown by MBE) that indicate an enhancement (of only ~2× in the exciton binding energy for L = 100 Å). The data of Fig. 6 and other low-level cw and laser data on rectangular cleaved samples indicate that the two-dimensional exciton can be involved in recombination in these quantum-well heterostructures.

In order to determine how closely the low-energy phonon-sideband laser modes observed in the data from the (1–7) 200-50-Å QWH (Figs. 3–6) are related to the confined-carrier transitions, a number of samples with a thicker GaAs layer substituted in place of the "large" L = 200-Å well have been employed. As the layer size L increases, the

FIG. 5. Comparison of the pulsed photoemission (300 K) of a rectangular sample [12 × 226 µm²] cleaved from a single 200-Å QWH with a rectangular sample [27 × 234 µm²] cleaved from the same QWH wafer as the samples of Figs. 3 and 4. The high energy emission of a single 200-Å QWH [2.9 × 10³ W/cm²] is cut off by the 7-well (L, ~ 50 Å) array of bi[17 × 10³ W/cm²].
behavior of the larger well shifts more toward bulk GaAs; the confined-carrier states then become very closely spaced and the \( n = 1 \) transition is very nearly degenerate with \( E_{g} \). The uncertainty in assigning an edge or origin for phonon-sideband laser operation is thus greatly decreased. This is the case for \( L_{31} \sim 500 \text{ Å} \).

An example of the emission spectra (77 K) of the (1–7) 500-50-Å QWH sample is shown in Fig. 7. The cw spectrum (curve a), \( 1.2 \times 10^{4} \text{ W/cm}^{2} \) exhibits laser operation on a phonon sideband of the \( n' = 1' \) transition of the 500-Å quantum well. Spontaneous emission peaks as seen in Figs. 3, 5, and 6 are also observed. At a pulsed excitation of \( 5 \times 10^{4} \text{ W/cm}^{2} \), curve b), the same sample lases strongly in the range of the phonon sidebands of the \( n = 1, 1', 2, 2', 3, \) and \( 3' \) transitions of the \( L_{31} \sim 500-\text{Å} \) layer. A narrower sample [curve c), \( 8 \times 10^{4} \text{ W/cm}^{2} \)], with higher cavity losses, is used to force laser operation up in energy to the lowest confined-carrier transitions to enable their identification.

A design modification on the (1–7) 500-50-Å QWH is achieved by introducing a second phonon-generating and reflecting array of seven \( L_{32} \sim 50-\text{Å} \) quantum wells on the other side of the \( L_{31} \sim 500-\text{Å} \) GaAs layer. The result is a (7–1–7) 500-50-50-Å structure in which \( 58\% \) of the GaAs in the active region is in the small-well array portion. Any reflection of LO phonons by the twin 50-Å well arrays should tend to localize the LO phonons in the vicinity of the \( L_{31} \sim 500-\text{Å} \) thicker layer and strongly affect the recombination radiation spectrum. Typical pulsed room-temperature photoluminescence spectra are shown in Fig. 8. The bars numbered 1–5 are the locations of the five lowest-energy electron-to-heavy-hole transitions of the 500-Å quantum well. At \( 10^{4} \text{ W/cm}^{2} \), curve a), laser threshold occurs \( \sim \hbar \omega_{LO} \) lower in energy than the \( n = 1 \) transition. Slight ringing is also observed in the energy range of the \( n = 2 \) transition. An increase in excitation level to \( 2 \times 10^{4} \text{ W/cm}^{2} \), curve b), results in intense laser operation on the phonon sideband of the lowest confined-particle transitions and also weaker laser modes between the \( n = 1 \) and \( n = 4 \) transitions. Note that the data of Figs. 7 and 8 exhibit laser operation \( \sim \hbar \omega_{LO} \) lower in energy than the lowest-energy laser emission expected due to band-to-band recombination in bulk, undoped GaAs. This emission occurs at a transition energy in which no states exist in these structures. As mentioned earlier, both of these samples are undoped \( n_{a} \). Therefore this laser operation is not impurity related, since \( \sim 10^{13} \text{ cm}^{-3} \) impurities are necessary for GaAs to lase on a band-to-impurity transition. The emission spectra of Figs. 7 and 8 establish that phonon-sideband laser operation can be achieved in a GaAs laser of nearly bulk dimensions \( \sim 500 \text{ Å} \) that is sandwiched between Al\(_{x}\)Ga\(_{1-x}\)As as confining layers.

Further increase in the size of the larger GaAs well in these coupled array heterostructures begins to decrease the effectiveness of the laser operation of the larger layer. For these heterostructures (inset of Fig. 3), as the single larger well \( L_{31} \) is increased in size from 200 to 500 to 1500 Å, the GaAs fraction in the active region represented by the \( L_{31} \sim 50-\text{Å} \) seven-well array decreases from 0.64 to 0.41 to 0.19. Assuming that this is roughly the percent of injected electrons that thermalize in the small-well array section, we expect the number of LO phonons generated by the seven well \( L_{31} \sim 50-\text{Å} \) array to decrease rapidly with increasing \( L_{31} \). Note that the fraction of electrons that recombine in the array is expected to be even less than the above estimate since carriers can tunnel into the larger GaAs layer and scatter to
still lower energy before recombining. Therefore, in spite of the fact that the small-well array contributes some recombination radiation, which can serve as a reference, this radiation is relatively weak and has little effect on the lasing behavior of the larger GaAs layer for $L_{d1} < 500 \text{Å}$. Pulsed room-temperature laser operation of the (1-7) 1500-50-Å QWH sample (iii) is shown in Fig. 9. Since the single $L_{d1} \sim 1500$-Å-GaAs layer (coupled to the $L_{d2}$ 50-Å array) is definitely in the bulk limit, only the GaAs energy gap $E_g$ is used as a reference for emission originating in the thick layer. The 1 and 1' bars near 8000 Å in Fig. 9 denote the energies of the first electron-to-light- and -to-heavy-hole transitions for carriers localized in the $L_{d2}$ ~ 50 Å seven-well multilayer. One interesting feature of the data in Fig. 9 is the relatively weak spontaneous emission peak located ~$\hbar\omega_{LO}$ lower in energy than the $L_{d2}$ ~ 50-Å multilayer transitions $n = 1$ and $n' = 1$. This emission is weak because of the small fraction (0.19) of the active region GaAs that is contributed by the 50-Å array. The most important feature of this sample is that it too lases at energies below $E_g$, as far below as ~$\hbar\omega_{LO}$. At 77 K this heterostructure lases at $E_g$ and also exhibits the higher-energy spontaneous reference peak of Fig. 9. This peak, however, is not shifted below the $L_{d2}$ ~ 50-Å $n = 1$ transition as it is at 300 K, but rather occurs very nearly on the $n = 1$ transition. That both the multilayer array and the larger-layer emission shift down in energy relative to their band-to-band transitions as the lattice temperature is increased indicates that the thermal LO-phonon occupation number is increased enough to cause both transitions to operate on phonon sidebands. A further experiment on a DH wafer with $L_d \sim 600$ Å (all layers undoped, $n_d - n_s \leq 10^{13}$ cm$^{-3}$) has exhibited a similar temperature dependence. Therefore laser operation at $\hbar\omega_0 - E_g = \hbar\omega_{LO}$ in a DH is considered as originating in phonon-assisted recombination. The thermal phonons present due to the lattice temperature (300 K) plus the nonthermal LO phonons generated during carrier relaxation are sufficient to produce phonon-sideband laser operation at the high injection levels characteristic of DH laser operation.

While the data of Fig. 9 indicate that phonon-sideband laser operation can be induced by changing the thermal LO-phonon occupation number, the spectra of Fig. 10 demonstrate that a similar result can be achieved by increasing the nonthermal phonon occupation number. The cw room-temperature laser spectra of Fig. 10 have both been obtained on samples from an $L_d \sim 50$-Å six-well, five-barrier ($x = 0.30$) QWH. This undoped multiple quantum-well active region ($n_d - n_s \leq 10^{13}$ cm$^{-3}$) is imbedded in an Al$_x$Ga$_{1-x}$As ($x \sim 0.32$)-$p$-$n$ junction. The (a) spectrum is from a portion of the wafer processed into simple stripe geometry diodes. In contrast, the (b) spectrum is from a smaller portion of the wafer from which both the $n$-type GaAs substrate and also the $p$-$+$GaAs contact layers have been removed. Note that the diode, 10(a), operates on the phonon-sideband of the $n' = 1'$ transition, while the photoexcited sample operates at

FIG. 8. Pulsed room-temperature laser operation of a rectangular (68 x 234 μm$^2$) QWH sample with an active region consisting of a 500-Å GaAs well sandwiched between two arrays of seven 50-Å GaAs wells all of which are coupled by 50-Å Al$_x$Ga$_{1-x}$As ($x \approx 0.32$) barriers. At 10$^4$ W/cm$^2$ as spontaneous emission is peaked in the range of the lowest transitions of the 500-Å well ($n = 1$) with laser modes developing one phonon below the $n = 1$ transition located almost at $E_g$. At 2 x 10$^4$ W/cm$^2$, the laser operation is well developed one phonon below the $n = 1$ transition for $E_g$; and weaker laser emission is observed between the $n = 1$ and $n = 4$ transitions of the 500-Å well.

FIG. 9. Pulsed room-temperature photoemission (3.6 x 10$^4$ W/cm$^2$) of a sample (43 x 94 μm$^2$) whose active region consists of a 1500-Å layer of GaAs (bulk dimensions) coupled to an array of seven 50-Å GaAs wells. The coupling barriers are 50-Å-Al$_x$Ga$_{1-x}$As ($x \approx 0.32$). A reference spontaneous spectral hump occurs between the 1-LO and 1'-LO transitions of the 50-Å array, and the sample lases in the range $\hbar\omega_{LO}$ below the energy gap of bulk material, indicating a phonon-assisted recombination. This contribution to emission in heterostructures with layers as thick as 1500 Å.
much lower energy, \( \sim 2 \hbar \omega_{\text{LO}} \) below the \( n = 1 \) transition. The important difference between the diode and the photo-

luminescence sample, other than the method of excitation, is the optical cavity size. The diode is 223 \( \mu \text{m} \) long, while the

photoexcited sample is 22 \( \mu \text{m} \) in width and has nearly ten times larger cavity end loss than the diode. Two factors enter

into the laser operation of very narrow samples: (1) bandfilling tends to increase the lasing energy, and (2) the increased density of electron-hole-pairs necessary to attain laser threshold gives rise to an increase in the nonthermal LO phonon occupation number made possible

by the higher laser threshold density induces lower-energy phonon-assisted laser operation, thus decreasing the lasing sational exciton transitions relative to

the emission into two peaks is due to the spatial separation of

the electron-hole pairs in the QWH (in \( L_1 \), and in \( L_4 \) because of spectral broadening) to lead to relatively ineffi-

cient laser operation of these structures. The broadening in the emission is decreased until finally the degenerate case

\( \lambda \sim 7600 \, \text{Å} \). This behavior is possibly due to the better phonon confinement that is believed to exist in a 50-Å-layer QWH as discussed below. It is interesting to compare this emission \( \lambda \), six-well, \( L_1 = 50 \, \text{Å} \) with that of the \( (1-7) \) 200-

50-Å structure, curve \( a \), which also contains a 50-Å multi-

layer array. Note that the spontaneous emission from the

multilayer array portion of curve \( a \), \( \lambda \sim 7800 \, \text{Å} \), is not as

low in energy as that from the degenerate case curve \( f \),

\( \lambda \sim 8000 \, \text{Å} \), indicating that the carriers in the \( (1-7) \) structure

are more likely to scatter to the 200 Å well than recombine on a sideband \( 2 \hbar \omega_{\text{LO}} \) lower in energy than the 50-Å \( n = 1 \) transitions.

An important feature of these spectra is that the existence of two peaks in the \( (1-7) \) and \( (1-6-1) \) QWH's are likely

(because of spectral broadening) to lead to relatively ineffi-
cient laser operation of these structures. The broadening of the emission into two peaks is due to the spatial separation of

the electron-hole pairs in the QWH (in \( L_{11} \), and in \( nL_{22} \)). This

broadened emission implies both a spatial and an energetic line broadening (an inhomogeneous line). As the \( L_{11} \) and \( L_{22} \) GaAs layer sizes are chosen to approach the same thickness \( (a) \) to \( (b) \) to \( (c) \), the broadening in the emission is decreased until finally the degenerate case \( (L_{11} = L_{22} = L_1; (d), (e), \) and \( (f) \) results. Thus while the case of nondegenerate structures can be designed to demonstrate LO-phonon effects and are interesting light emitters, their usefulness as efficient lasers is questionable because the emission linewidth is artificially broadened.

IV. DISCUSSION

A complete theoretical description of the effects described above is difficult for several reasons. For example, not much is known about the mean free path of phonons under the condition of high excitation, or about multiphonon emission, or in general about indirect optical transitions in a direct semiconductor. Usually it is agreed that indirect transitions, i.e., transitions involving phonons and photons, are negligible in direct materials if the electron-phonon coupling constant is small as it is in GaAs. This

---

05b et al. 965
phonon coupling constant,7 and the high-power densities "compressed" into a relatively small volume 2,10,28 (the QWH active region). Below we describe the criteria that have guided the choice of the sample geometry.

In spite of the fact that not much is known about phonon-phonon interactions, the phonon mean free path at high excitation levels, and the direction of maximum emission intensity, we assume that layers with dimensions of a multiple of the phonon wavelength at the maximum phonon intensity would reflect and confine most. The wavelength of maximum intensity of phonons emitted perpendicular to the layers can be determined in the following way: Previous calculations9 show that the emission probability for phonons (perpendicular to the layers) is a monotonically decreasing function of q if free-carrier screening is not taken into account. A two-dimensional analysis shows that all wavelengths longer than \(2\alpha_q = 160\,\text{Å}\) are effectively screened, where \(\alpha_q\) is the effective Bohr radius. Therefore we expect a maximum in the phonon intensity at wavelengths near \(2\alpha_q\). The emission probability parallel to the layers (again for quasi-two-dimensional electrons) shows two distinct peaks.8

The peak at the longer wavelength is again almost certainly screened. The peak at the shorter wavelength occurs as given in Ref. 8 at

\[
q = 2.52 \times 10^{-6}\,\text{m}^{-1/2} \left[1 - (1 - 1/m)_{1/2}\right]\,\text{cm}^{-1}.
\]

Here we have used the material constants of GaAs. The integer \(m\) corresponds to the energy \(m\hbar\omega_\text{LO}\) above the bottom of the quantum-well subband from where the electron cascades downward in thermalizing. Using the above expression, we obtain as a typical wavelength and thus layer or well size the values shown in Table I. These values have been used as guidelines in the choice of sample dimensions.

V. CONCLUSIONS

A series of experiments have been described above to determine the extent of LO-phonon contribution to metalorganic chemical vapor deposited Al\(_x\)Ga\(_{1-x}\)As-GaAs quantum-well-heterostructure (QWH) laser operation. The undoped photoluminescence structures studied have active regions consisting of a large GaAs quantum well \((L_{\text{d}1})\), or in some cases a bulk layer \((L_{\text{d}2} > 500\,\text{Å})\), coupled to a small-well \((L_{\text{d}3})\) multilayer array. Phonons generated during carrier

<table>
<thead>
<tr>
<th>(m)</th>
<th>(\lambda = 2\pi/q) (Å)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>250</td>
</tr>
<tr>
<td>2</td>
<td>103</td>
</tr>
<tr>
<td>3</td>
<td>79</td>
</tr>
<tr>
<td>4</td>
<td>67</td>
</tr>
<tr>
<td>5</td>
<td>58</td>
</tr>
<tr>
<td>6</td>
<td>53</td>
</tr>
<tr>
<td>7</td>
<td>49</td>
</tr>
<tr>
<td>8</td>
<td>45</td>
</tr>
<tr>
<td>9</td>
<td>42</td>
</tr>
<tr>
<td>10</td>
<td>40</td>
</tr>
</tbody>
</table>

argument does not hold for high excitation levels since the average phonon occupation number which appears in the matrix elements for indirect transitions increases rapidly, resulting in a high "effective" electron-phonon interaction.

This should be generally true and the effect should give important contributions to the optical constants under high excitation conditions, for example, as encountered in the parallel case of laser annealing. Before describing our choice of sample geometries to enhance the phonon effects, we would like to emphasize that previous studies have shown that size-quantization effects tend to favor a nonthermal phonon occupation. This occurs because of the two-dimensional density of states, a slight increase in the electron-
thermalization in the multilayer array have been shown to induce phonon-sideband laser operation of the larger GaAs layer. In undoped structures with the large-well dimension $L_{w} \sim 500 \AA$, the phonon-sideband emission is in the range $\hbar \omega - E_g - \hbar \omega_0$, that is, the emission is $\hbar \omega_0$ lower in energy than the lowest transition allowed in bulk undoped GaAs. Phonon-sideband laser operation has been shown to be induced by an increase in either the thermal or the non-thermal LO-phonon occupation number. In fact, the increase in the thermal phonon occupation number at 300 K over that at 77 K has been shown to result in phonon-sideband laser operation of a bulk GaAs active layer in the size range of standard double heterojunctions ($L_{w} \sim 1500 \AA$). While these heterostructures, which contain a large quantum well coupled to a thin multilayer array, are useful in understanding phonon-sideband laser operation, they are not likely to be the most efficient lasers because of the artificially created line broadening resulting from two different quantum-well sizes. The MO-CVD QWH wafers used in this work have been designed to optimize the auxiliary phonon-generating and -reflecting arrays coupled to the larger GaAs quantum-well active layers. The optimization has been accomplished by choosing the array layer size equal to the wavelengths of the phonons with maximum emission probability.

ACKNOWLEDGMENTS

The authors are grateful to Yuri S. Moroz, R. T. Gladin, B. L. Marshall, and B. L. Payne (Urbana) for technical assistance, and to G. E. Stillman for helpful discussions. The work of the Illinois group has been supported by NSF Grants DMR 79-09991 and DMR-77-23999 and Navy Contract N00014-79-C-0768; the work of the Rockwell group has been partially supported by the Office of Naval Research, Contract N00014-78-C-0711.

Alloy Clustering in Al$_{1-x}$Ga$_x$As-GaAs Quantum-Well Heterostructures

N. Holonyak, Jr., W. D. Laidig, and B. A. Vojak

Department of Electrical Engineering and Materials Research Laboratory, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801

and

K. Hess

Department of Electrical Engineering and Coordinated Science Laboratory, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801

and

J. J. Coleman and P. D. Dapkus

Rockwell International, Electronics Research Center, Anaheim, California 92803

and

J. Bardeen

Department of Physics, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801

(Received 28 July 1980)

Data on spontaneous and stimulated emission, in the photon-energy range $E_g + 5\Delta E_{LO} \geq h\nu \geq E_g$, are presented on Al$_{1-x}$Ga$_x$As-GaAs quantum-well heterostructures with Al$_{1-x}$Ga$_x$As $(x = 0.4 - 0.5)$ coupling barriers of size $L_b \sim 40 - 70$ Å and GaAs wells of size $L_a \sim 30 - 40$ Å. For $L_a, L_b \sim 50$ Å, Al-Ga disorder (clustering) in the alloy barriers is consistent with the observed spectral broadening and downward energy shift of the confined-particle transitions. A simple substitution of binary (AlAs) for ternary (AlGaAs) barriers eliminates alloy clustering and its effects, and makes unambiguous the identification of clustering in alloy barriers.

PACS numbers: 73.40.Lq, 71.50.+t, 78.45.+h

In contrast to earlier work, stimulated emission has been observed recently at energy $5\Delta E_{LO}$ to $6\Delta E_{LO}$ below the confined-particle transitions of Al$_{1-x}$Ga$_x$As-GaAs multiple-quantum-well heterostructures (QWH) with narrow wells ($L_a \leq 50$ Å) and narrow alloy barriers ($L_b \leq 50$ Å). An example is illustrated in Fig. 1, a. The lowest energies are a little above that of the GaAs energy gap, $E_g$. With increased pump power, stimulated emission is transferred to the neighborhood of the confined-particle states [Fig. 1, b]. In this paper, we show that because of disorder and clustering in the narrow ternary barriers (which can be removed by the use of binary barriers, AlAs), a continuum of states may exist in the QWH, the lowest with energies extending down to the band edge of pure GaAs. It is suggested that real phonon transitions take the electrons down to these levels, from which stimulated emission then occurs. With higher power, emission from the confined-particle states is enhanced and electrons do not have time to cascade to the lower levels.

The Al$_{1-x}$Ga$_x$As-GaAs quantum-well heterostructures of interest here are grown by metalorganic chemical vapor deposition. Gas flow rates and layer growth times are electronically controlled to ensure layer reproducibility. Growth rates are controllable in the range 2 - 50 Å/sec for GaAs and in the range 2.5 - 100 Å/sec for AlGaAs $(x \sim 0.40)$, which makes it practical to grow layers as thin as 10 Å. The first layer grown on the GaAs substrate is a GaAs buffer layer to provide a good crystallographic surface for the confined-particle states. This is followed by the QWH active region, which consists of a series of GaAs quantum wells and Al$_{1-x}$Ga$_x$As (or AlAs) barrier layers. The final layer is a second relatively thick (- 0.50 μm) Al$_{1-x}$Ga$_x$As $(x \sim 0.50)$ confining layer. This is followed by the QWH active region, which consists of a series of GaAs quantum wells and Al$_{1-x}$Ga$_x$As (or AlAs) barrier layers. The final layer is a second relatively thick (- 0.50 μm) Al$_{1-x}$Ga$_x$As $(x \sim 0.50)$ confining layer. All layers are undoped $(n_a - n_x < 10^{15}/$cm$^3$). Samples for photoluminescence experiments are prepared by polishing and selectively etching off the GaAs from the substrate side. Cleaved portions (20 - 100 x 100 - 300 μm$^2$) of the remaining thin wafer (- 1.3 μm thick) are imbedded for neat sinking into In under a sapphire window (77-K experiments) or into annealed Cu under a diamond window (300-K experiments). and are photooxidized with an Ar$^+$ (5145 Å) or a dye-tunable (6540 Å)
laser.

The 300-K laser data of Fig. 1 demonstrate the range of laser mode energies attainable from a QWH with an active region consisting of six \( \sim 30 \) \( \text{Å} \) GaAs quantum wells coupled by five \( \sim 50 \) \( \text{Å} \) \( \text{Al}_{x}\text{Ga}_{1-x} \text{As} \) \( (x \sim 0.40) \) barriers. The 1 and 1' markers indicate the allowed electron-to-heavy-hole and electron-to-light-hole transitions, respectively, for \( 30 \) \( \text{Å} \) wells separated by perfect 50-\( \text{Å} \) barriers (i.e., no alloy clustering). The 1 and 1' (110) markers indicate the lowest transitions of a 110-\( \text{Å} \) well. Typical cw laser operation (\( b, 4.8 \times 10^3 \text{ W/cm}^2 \)) occurs slightly below the 1 (110) marker, while the spontaneous background extends to higher energy. Pulsed operation of a narrower sample \( \varnothing, 6.8 \times 10^4 \text{ W/cm}^2 \) produces lasing at the expected energy of the \( n = 1 \) transition (30-\( \text{Å} \) well).

![Diagram of laser emission and energy transitions](image)

**FIG. 1.** Laser spectra (300 K) of a photopumped QWH grown by metalorganic chemical vapor deposition with an active region consisting of six \( \sim 30 \) \( \text{Å} \) GaAs wells and five \( \sim 50 \) \( \text{Å} \) \( \text{Al}_{x}\text{Ga}_{1-x} \text{As} \) \( (x \sim 0.40) \) barriers. The 1 and 1' markers indicate the allowed electron-to-heavy-hole and electron-to-light-hole transitions, respectively, for \( 30 \) \( \text{Å} \) wells separated by perfect 50-\( \text{Å} \) barriers (i.e., no alloy clustering). The 1 and 1' (110) markers indicate the lowest transitions of a 110-\( \text{Å} \) well. Typical cw laser operation (\( b, 4.8 \times 10^3 \text{ W/cm}^2 \)) occurs slightly below the 1 (110) marker, while the spontaneous background extends to higher energy. Pulsed operation of a narrower sample \( \varnothing, 6.8 \times 10^4 \text{ W/cm}^2 \) produces lasing at the expected energy of the \( n = 1 \) transition (30-\( \text{Å} \) well).

The locations of the confined-carrier states of this QWH system are labeled in Fig. 1. The location (energy) of these states is expected to be different for different wavelengths and is labeled in the figure by the yellow marker, with the expected energy spectrum of this quantum system. For example, the \( n = 1 \) confined-electron state shifts downward by \( \sim 140 \text{ meV} \) for a size shift from \( L, \sim 30 \text{ Å} \) to \( L, +L_b + L_s, \sim 110 \text{ Å} \). The location (energy) of the lowest confined-carrier transitions of a \( \sim 110-\text{Å} \) GaAs quantum well are also labeled in Fig. 1. Note that alloy clustering in the barrier layers sufficient to create GaAs paths through the \( \text{Al}_{x}\text{Ga}_{1-x} \text{As} \) barriers is expected to have a drastic effect in broadening and lowering the energy spectrum of this quantum system. For example, the \( n = 1 \) confined-electron state shifts downward by \( \sim 140 \text{ meV} \) for a size shift from \( L, \sim 30 \text{ Å} \) to \( L, +L_b + L_s, \sim 110 \text{ Å} \).

A result of this shift is that the density of states of a QWH with alloy clustering in the barriers will not exhibit an abrupt step to zero at energies below the lowest confined-particle states of an ideal structure. Instead, the density of states is expected to be small but significant below these "lowest" confined-carrier states, and then drop to zero for energies less than \( E_s(\text{GaAs}) \). Besides depending upon the barrier size \( L_b \), the exact form of the density of states will depend on the average cluster size, the form of the cluster size distribution, and on the composition \( x \) of the \( \text{Al}_{x}\text{Ga}_{1-x} \text{As} \). Also, cluster-induced quantization in the \( x,y \) dimensions will play a role.

These additional lower-energy states are expected to play an important part in radiative emission from a QWH. The existence of small areas or patches within the active region with lower-energy states (areas that increase in number with the number of barriers) increases the probability of LO-phonon-assisted recombination processes at energies \( E_{11} < E_{1} < E_s \), since virtual transitions are no longer required. Instead, real transitions in this range at multiples of \( \hbar \omega_{11} \) below the \( n = 1 \) and \( n' = 1' \) transitions of the \( L_s, \sim 30 \text{ Å} \) well are possible.
Further evidence for alloy clustering in the Al$_{1-x}$Ga$_x$As barriers is shown (Fig. 2) by the form of the high-level spontaneous emission spectra of a two-well, one-barrier ($x=0.5$) QWH (a different QWH wafer) with all three layers $\sim 40$ Å thick. Note that in this case the barrier size is smaller ($40$ Å) and approaches and helps identify the average cluster size. As in Fig. 1, the confined-carrier transitions of the small quantum well and also of the larger $L_x + L_y + L_z \sim 120$ Å composite quantum well are labeled in Fig. 2. The two samples ($a, 4 \times 10^4$ W cm$^{-2}$, 90 $\times 360 \mu$m$^2$; $b, 10^5$ W cm$^{-2}$, $56 \times 195 \mu$m$^2$) exhibit very similar spectra as, in fact, do all of the samples from this wafer. A large peak in the range of $n'=1'$ is observed. The emission does not drop to zero just below the $n=1$ $e^{-h\bar{v}}$ transition, as would be expected in the ideal cluster-free limit, but extends downward in energy to nearly the location of the $n=1$ (120) and $n'=1'$ (120) transitions, which are near a distinct shoulder in the emission. An increase in the barrier thickness to $\sim 70$ Å results in cutoff of most of this lower energy emission. As the barrier thickness $L_x$ is decreased from $\sim 70$ Å (Ref. 9) to $\sim 50$ Å (Fig. 1) to $\sim 40$ Å (Fig. 2) and approaches the average cluster size, tunneling filaments are likely to appear in the Al$_{1-x}$Ga$_x$As barriers, which results in a major increase of the effective well dimension from $-L_x$ to $-L_x - L_y - L_z$. The observation of spectra such as those of Fig. 2 allow an estimate to be made of the cluster size ($\sim 40$ Å).

Further $300$-K laser data on a 29-barrier, 30-well $L_x \sim 30$ Å, $L_y \sim 50$ Å superlattice structure (not shown) demonstrate that laser operation below $E_g$ is also attainable. This fact, along with recent laser data on QWH's consisting of a large quantum well (or in some cases a bulk layer) coupled to a phonon-generating and -reflecting array of smaller quantum wells, indicate that virtual phonon-assisted recombination processes with $n < E_g$ can occur and are not inconsistent with the present data. Alloy clustering (in ternary barriers), however, allows actual states to exist between the bulk band edge and the lowest quantum states characteristic of an ideal QWH and thus permits real phonon processes to scatter the electrons to lower energies before recombining.

It is worth mentioning that a reinterpretation of previous investigations of disorder scattering indicates that cluster models might have to be involved to explain successfully the experimental results for electron mobilities in III-V alloys. For example, negligible alloy scattering seems to exist in In$_{0.5}$Ga$_{0.5}$As and strong alloy scattering in the quaternary system In$_{0.5}$Ga$_{0.5}$P$_{0.1}$As$_{0.9}$, which (for the latter) cannot be explained on the basis of random-compositional-disorder models alone. In addition, these models do not take into account, in detail, the peculiarities of crystals such as Al$_{1-x}$Ga$_x$As or GaAs$_{1-x}$P$_x$ that undergo a direct-indirect transition in the range $x=x_c=0.4-0.5$, nor whether such crystals are particularly prone to clustering. It is also worth mentioning that data are not presently available indicating how sensitive cluster formation is to the specific process (vapor-phase epitaxy, liquid-phase epitaxy, molecular-beam epitaxy) used to grow a III-V alloy.

In any case, the basic features of the Al$_{1-x}$Ga$_x$As alloy clustering described above are clear since, besides the data of Figs. 1 and 2, simple substitution of binary barriers (including very narrow barriers, $\sim 10$ Å) for the ternary barriers employed here eliminates recombination below the expected (ideal) confined-particle transitions of a QWH. These further data are shown in Fig. 3, which is for the case of a QWH with twelve GaAs wells ($L_x \sim 50$ Å) interleaved in the active region with thirteen binary (nonclustered) AlAs barriers ($L_y \sim 10$ Å). The laser operation of the sample ($50 \times 90 \mu$m$^2$) occurs exactly on the $n=1,$
and stimulated emission only at the 50-Å GaAs wells. The excitation power densities are high (\(10^5\) W/cm\(^2\)) since absorption of the incident pump beam (\(\lambda_p \approx 6540\) Å) occurs only at the 50-Å GaAs wells. Spontaneous (\(\sigma\)) and stimulated \(\sigma^\prime\) emission occur only on the \(n=1\) and \(n'=1\)' transitions, and not at lower energy as in Figs. 1 and 2.

FIG. 3. Photoluminescence (laser) spectra (77 K) of a QWH sample with an all-binary (cluster-free) active region consisting of twelve \(\sim 10\)-Å AlAs barriers. The excitation power densities are high (\(10^5\) W/cm\(^2\)) since absorption of the incident pump beam (\(\lambda_p \approx 6540\) Å) occurs only at the 50-Å GaAs wells. Spontaneous (\(\sigma\)) and stimulated \(\sigma^\prime\) emission occur only on the \(n=1\) and \(n'=1\)' transitions, and not at lower energy as in Figs. 1 and 2.

Finally we emphasize that the consequences of alloy clustering are very different for QWH layers and for bulk semiconductors. In a bulk III-V alloy the changes in the scattering rates (e.g., decrease in carrier mobility) due to clusters are quite small, whereas in layered structures size-quantization effects can be totally destroyed. It is exactly these effects of size quantization that are probed with QWH laser emission, which is therefore a sensitive new tool to investigate clustering.

The authors are grateful to Yuri S. Moroz, R. T. Giadin, B. L. Marshall, and B. L. Payne (Urbana) for technical assistance, and to G. E. Stillman for various discussions. This work has been supported by the National Science Foundation under Grants No. DMR-79-09991 and No. DMR-77-23999 and by U. S. Navy Contract No. N00014-79-C-0768; the work has also been partially supported by the U. S. Office of Naval Research under Contract No. N00014-78-C-0711.

Although confined-carrier as well as photon-assisted recombination transitions have been identified in the emission spectra of quantum-well heterostructures (QWH) lasers, a number of unexplained emission peaks still remain. While the phonon-sideband laser operation occurs at or even 2x36 meV lower in energy than the lowest (n=1) confined-particle transitions (n=a=1), other spontaneous and stimulated peaks have been observed in the range (20 meV) between the phonon peaks and the lowest confined-carrier transitions. In the present work low temperature (4.2-77 K) photoluminescence and laser data on metal-organic chemical vapor deposited AlGaAs-GaAs quantum-well heterostructures indicate the involvement of the two-dimensional exciton in recombination in quantum-well heterostructures.

Low temperature (4.2-77 K) photoluminescence and laser data on metal-organic chemical vapor deposited AlGaAs-GaAs quantum-well heterostructures are presented that exhibit emission peaks between the lowest energy confined-carrier transitions and their phonon sidebands. These data indicate the involvement of the two-dimensional exciton in recombination in quantum-well heterostructures.

E_{\text{QWH}} = h(13.6/k^2)(\mu/\mu_0) \text{eV},

where \(1/\mu = (1/\mu_e) + (1/\mu_h)\).
RECOMBINATION IN QUANTUM-CELL HETEROSTRUCTURES

Vol. 35, No. 6

Energy (eV)

\(1.50\)
\(1.54\)
\(1.58\)

\(\text{Al}_x\text{Ga}_{1-x}\text{As-GaAs (5 + 6)}\)
\(x \sim 0.27\)
\(L_x \sim 120\,\text{Å}\)

\(4.2\,\text{K}\)

Intensity

Fig. 1 Photoluminescence spectra (4.2 K) of an \(\text{Al}_x\text{Ga}_{1-x}\text{As-GaAs multiple-quantum-well heterostructure grown by metalorganic chemical vapor deposition. The active region, sandwiched between two \(\text{Al}_x\text{Ga}_{1-x}\) As (x=0.42) confining layers, consists of six 120 \(\text{Å}\) GaAs wells separated by five 120 \(\text{Å}\) \(\text{Al}_x\text{Ga}_{1-x}\) As (x=0.27) barriers. Low-level CW emission (10\(^2\) W/cm\(^2\), curve a) occurs primarily at energies below those of the lowest confined-particle transitions indicated on the horizontal axis by the heavy (n=1, e=hh) and light (n'=1', e=th) markers. At slightly higher CW excitation (6.6x10\(^2\) W/cm\(^2\), curve b) stimulated emission occurs at LO-phonon energy (\(h\omega_{\text{LO}} = 36\,\text{meV}\)) below the n'=1' e=th transition, as indicated by the LO label. With pulsed excitation (6.6x10\(^3\) W/cm\(^2\), curve c) the emission spectrum from the same sample shows structure at still lower energy. The arrows marked A and B designate energies 20 meV below the n=1 e=hh transition energy and 11 meV below the n'=1' e=th transition energy, respectively. Similarly, the arrows marked A-LO and B-LO correspond to energies 36 meV below those designated by the A and B arrows.)
Values of the parameters used are: \( n^* = 0.45 \), \( m^* = 0.087 \), \( n^0 = 0.0065 \), \( \alpha = 12.6, 15 \) for the relative static dielectric constant \( \epsilon \). The location of the two emission peaks \( A \) and \( B \) are in very close agreement with the calculated two-dimensional exciton energies. Note that two separate exciton peaks are expected in this case since \( k_x = k_y = 0 \) (for \( n = 1 \)) the light- and heavy-hole valence bands are not degenerate as they are at \( k = 0 \) in the bulk limit. That the light-hole exciton location is in better agreement with the estimate than that of the heavy hole could be due to the difference in the extent of their two-dimensionality. An electron-heavy hole exciton has a bulk Bohr radius of -120 Å while the electron-light hole exciton has a bulk Bohr radius of -170 Å. The light-hole exciton is thus expected to be closer to the two-dimensional limit than the heavy-hole exciton. The low energy shoulder observed on curve c of Fig. 1 (between arrows A-LO and B-LO) is in the range \( h_0 \) below the \( A \) and \( B \) emission peaks and could be a phonon sideband of the exciton emission since it appears only at higher excitation level when the phonon density is expected to be quite high.

Emission spectra from the second wafer, which is designed with a 7-well phonon-generating array (7 \( L = 50 \) Å GaAs wells) coupled to a single large well \( L = 200 \) Å, are shown in Figs. 2 and 3. At low excitation level (Fig. 2a, 10 W/cm²), a spontaneous peak is observed \( h_0 \) below the \( n = 1 \) transitions of the 50 Å wells, which are degenerate with the \( n' = 3 \) transition of the 200 Å well. Another peak, the main peak, occurs at 1-8260 Å with a shoulder at 1-8280 Å that previously has not been identified. Upon increased excitation of the sample, curve b, laser operation occurs.

**Fig. 2** Comparison of CW (10 W/cm²) and pulsed (2.5x10⁵ W/cm²) emission spectra (77 K) of a photopumped multiple-quantum-well heterostructure with an active region composed of one 200 Å and seven 50 Å GaAs wells coupled by seven 50 Å AlGaAs \( x = 0.32 \) barriers. Note the shoulder (curve a) near the \( A \) arrow, which is located 20 meV below the lowest confined-particle transition \( n = 1, \epsilon hh \) of the 200 Å well. Pulsed excitation of the same sample (curve b) results in narrowly spaced end-to-end laser modes (not resolved in this curve) at \( h_0 \) phonon energy below the \( n = 1, \epsilon hh \) transition, and widely spaced edge-to-edge modes at approximately the same energy as the shoulder (and the \( A \) arrow) observed on curve a.
Fig. 3 Stimulated emission (77 K) of a sample obtained from the same wafer described in Fig. 2. The relatively high-level pulsed excitation (10^5 W/cm^2) produces emission in the energy range between the lowest confined-particle transitions (n=1 and n'='l') and an LO phonon energy below these transitions, allowing observation of two distinct sets of modes. The narrowly spaced end-to-end modes labeled by \( \Delta \lambda_1 \) (corresponding to the sample length, 160 \( \mu \)m) occur at energies in a region of very low absorption. For emission at energies higher than 20 meV below the n=1 e-hh transition (\( \Delta \lambda \) arrow), absorption is stronger in the region of the two-dimensional exciton, resulting in the widely spaced edge-to-edge laser modes labeled by \( \Delta \lambda_2 \) (corresponding to the sample width, 46 \( \mu \)m).

on a phonon sideband of the n'=l' transition of the 200 \( \AA \) quantum well and also 20 meV below the n=1 transition (modes A). Although the mode detail is not resolved in the figure, the phonon sideband (\( \Delta \lambda \)-LO, largest peak) lases in the lengthwise cavity (narrowly-spaced modes), while the laser operation at A occurs in the edge-to-edge direction of the rectangular sample. This difference in cavity oscillation for a rectangular sample, excited fully across its width but not entirely along its length, is consistent with \( \sigma(E_n) > \sigma(E_{n'='l'}, -\hbar \omega_{LO}) \). Since the stimulated emission on peak A occurs at \( E_A < E_{\lambda} \), the origin of this emission cannot be confused with confined-carrier transitions, which are all above \( E_{\lambda} \) and have been positively identified in other work. At very high excitation levels, excitons are not expected to exist in simple form. At large power densities, phonon effects are expected to be large, and emission below the confined-particle transitions is due mainly to phonon-shifted recombination from the lowest energy portions of...
the n=1 subband of the 200 Å well.9 This does not mean that exciton absorption in the unpumped regions of the sample can have no effect on laser operation. For example, Fig.3 shows the high level laser operation of a rectangular sample from the same wafer as that of Fig.2 (similar excitation). A continuous set of laser modes is observed in the 36 meV range from the n=1 transition of the 200 Å well down to the phonon-sideband of the n=1 transition. Note, however, that the cavity oscillations switch rather abruptly from narrowly spaced modes (Ax) to widely spaced modes (Ax) at an energy slightly higher than but very near A (i.e., -20 meV below the n=1 confined-carrier transition). The closely spaced modes Ax identify laser oscillations along the length of the sample while the broader spaced modes Ax are due to oscillations across the width. This switch in the cavity oscillations is an indication of a step in the absorption of the unexcited portion of the sample.

The type of mode behavior shown in Fig.3 in the range 20 meV below the lowest confined-carrier transition (n=1) has been observed also on samples from other QW wafers. With slight modification of the pumping beam geometry relative to the sample, particularly for a single 200 Å GaAs well,10 this behavior can be observed to extend up to the n=1 confined-carrier transition, presumably due to less absorption on the exciton compared to the first subband. For the samples of the present work (Figs. 2 and 3), it should be noted that the phonon generation in the 7-well array is very efficient,9 more so than for a single 200 Å GaAs quantum well. Thus resonant enhancement involving LD phonons should be quite significant in the range between the two-dimensional exciton and the first confined-carrier subband of the auxiliary 200 Å GaAs well, which is closely coupled to the phonon-generating array.

Two more items are worth mentioning: The "P" labels in Fig.1-3 are merely references. We know from other work that by simply reducing the GaAs well size the recombination at E2 can be cut-off but not the -20 meV band of recombination radiation located just below the lowest confined-particle transitions. The second is that for a variety of reasons the exciton band below the lowest recombination transitions (1, 1') is not expected to be as narrow or as sharp as for the bulk crystal case. Various scattering and relaxation processes over a considerable energy range play a role, as well as poorly understood high-density particle interactions. In addition, the particle distribution across the GaAs well is not uniform nor the effect of the confining layers, and thus the degree of two-dimensional shift in exciton binding energy. Also, if coupled wells are employed, they are not expected to be totally identical. Nor are the wells (single or multiple) necessarily entirely planar. Finally, it is worth mentioning that the narrowest QHR recombination lines are observed on phonon sidebands (E2-hA0 - E1-hA0) of the lowest confined-particle transitions.

The authors wish to thank Yuri S. Moroz, R.T. Gladin, B.L. Marshall, and B.L. Payne (Urbana) for technical assistance, and G.E. Stillman for various discussions. The work of the Illinois group has been supported by NSF Grants DMR 79-09991 and DMR 77-23999, and Navy Contract N00014-79-C-0731; the work of the Rockwell group has been partially supported by the Office of Naval Research, Contract N00014-78-C-0711.

REFERENCES

TEMPERATURE DEPENDENCE OF THRESHOLD CURRENT FOR A QUANTUM-WELL HETEROSTRUCTURE LASER

K. HESS, B. A. VOJAK, N. HOLONYAK, JR. and R. CHIN
Department of Electrical Engineering, University of Illinois, Urbana-Champaign, Urbana, IL 61801, U.S.A.

and

P. D. DAPKUS
Rockwell International, Electronic Devices Division, Electronics Research Center, Anaheim, CA 92803, U.S.A.

(Received 1 October 1979; in revised form 5 December 1979)

Abstract—The threshold current density, \( J_{th} \), of a quantum-well laser diode is calculated taking into account the quasi-two-dimensional nature of the heterostructure. The calculated value of \( J_{th}(T) \) for a quantum-well laser diode is found, in agreement with experiment, to be less temperature sensitive than that of a conventional double heterojunction laser. The step-like densities of states and the perturbed (hot) carrier distribution of a quasi-two-dimensional structure are responsible for the weaker temperature dependence. Supporting data on quantum-well AlGaAs-GaAs heterostructure laser diodes grown by MO-CVD are presented showing that in the conventional expression \( J_{th}(T) = J_{th}(0) \exp (T/T_0) \), \( T_0 \) can be as high as 437°C.

INTRODUCTION

Although the study of quantum size effects (QSE) in solids[1], including semiconductors[2], is not particularly a new area of investigation, quantum-well laser diodes (which exhibit QSE) have existed only since 1977[3]. Two kinds of quantum-well heterostructure laser diodes have been constructed, the first in the InP-In\(_x\)Ga\(_{1-x}\)As system[3, 4] and the second in the more highly developed AlGaAs-GaAs system[5-7]. In the case of the latter, continuous room temperature (CW, 300°K) laser operation has been achieved in both single[6] and multiple-quantum-well heterostructures[7], which, with promising reliability data[8], indicates that this form of laser diode is practical and more than a curiosity.

The quasi-two-dimensional nature of quantum-well heterostructures introduces several unique features to semiconductor laser operation: A step-like density of states replaces the usual bulk-crystal parabolic density of states, and phonon participation in recombination, which is not important below the bulk-crystal band edge, plays an observable role in quantum-well lasers[9, 10]. Among other effects, the step-like density of states of a quantum-well heterostructure changes the basic form of the current threshold for laser operation. Experimental data show that the current threshold, \( J_{th}(T) \), of a quantum-well laser diode is less temperature sensitive than that of the typical double heterojunction[7, 11]. In this paper the step-like density of states of a quasi-two-dimensional heterostructure is shown to be the basis of this improved temperature behaviour.

The temperature dependence of threshold current density is sensitive to both the form of the density of states and the carrier (electron and hole) distribution functions. Previous analyses of \( J_{th}(T) \) have employed a parabolic density of states[12] to model a bulk semiconductor while band tail effects have been incorporated in the form of a Gaussian[13] or exponential[14] distribution. Fermi–Dirac carrier distributions have been used in previous analyses. The use of a quasi-two-dimensional active region in a laser diode produces fundamental changes in this model. Below expressions for the temperature dependence of \( J_{th} \) for a quantum-well heterostructure are determined assuming a constant density of states in the limits of strong and weak electron–electron interactions. Experimental evidence for the weak dependence of \( J_{th} \) on temperature is presented for single-quantum-well heterostructure diodes with GaAs regions of thickness \( L \sim 200 \) Å.

MODEL

The electronic energy spectrum of a confined carrier in a thin GaAs layer sandwiched between AlGaAs confining layers has been shown by absorption measurements[15] to correspond to that expected of a one dimensional finite square potential well defined by the GaAs and AlGaAs band edges. Additionally, and of more importance to this work, radiative recombination from the lowest confined-particle transitions of a quantum-well heterostructure can be moved up in energy as high as \(-\sim 150 \) meV above \( E_0 \sim 1.6 \) eV, which agrees with calculations[16]. The parabolic energy-band dispersion in the x-y plane normal to the direction of quantization results in a constant density of states

\[
\epsilon_{\text{ex}} = m^* \omega^2/(\pi \hbar^2 L_x)
\]

for each subband. As shown in Fig. 1, the first step in the density of states begins at the lowest confined-electron state and is followed by another subband (step) with a constant (upward, \( E \uparrow \)) block of states, etc. This behaviour also applies to heavy holes and to light holes (\( E \downarrow \)) as is clear from the lower part of Fig. 1.

The energy distribution of electrons in the quantum well during laser operation is difficult to calculate. Electrons (and holes) cascade down (up) the quantum well by phonon emission and thermalize by electron-
gives and valence band edge for an AI,Ga,-,As-GaAs quantum-well heterostructure. The hole quasi-Fermi level.

Modeling these spikes as delta functions results in the cascading downward by emission of LO phonons is important.) These spikes should form for the distribution function composed of "spikes" where $n$ is the electron density in the well. The solid lines represent the least square fit of the data to the expression $J_d(T) = J_{d0}(0) \exp(-E_{L0}/kT)$. The device of curve (a) demonstrates that values of $T_n$ as high as 437°C are possible in quantum-well diodes. The decreased temperature dependence of $J_d$ in all three diodes is consistent with calculated expressions for $J_d(T)$.
the hole temperature would give only more complicated expressions and no important new features. Therefore we assume \( T_h = T_e \).

Using the densities of states and distribution functions described above, we calculate (assuming \( \Delta n = 0 \) transitions) the net rate of stimulated emission, \( r_s(E) \), and the rate of spontaneous emission, \( r_p(E) \), using the "no k-selection-rule" model of Lasher and Stern[12]. Thus

\[
r_s(E) = kT_e B \int_{E_{eh}}^{E_{el}} \degg(e) g_e(e-E) [f(e) - f_s(e-E)] \, \mathrm{d}E
\]

(6)

\[
r_p(E) = kT_e B \int_{E_{eh}}^{E_{el}} \degg(e) g_e(e-E) \times [1 - f(e-E)] f_s(e) \, \mathrm{d}E
\]

(7)

\[
R_m = kT_e \int_0^\infty E \, \degg(E) \, \mathrm{d}E
\]

(8)

where \( B \) is related to the average of the matrix element squared, \( E_{el} \) is the energy difference between the lowest energy confined-electron and confined-hole states, and \( E \) is the photon energy.

### ANALYSIS

Following the method of Adams[14], we begin with the rate equations for the electron density, \( n \), and the number of photons, \( N_{\omega} \), in the \( m \)th lasing mode or

\[
dn/dt = J(I|eL|) - R_p n - m N_{\omega} r_s(E_{\omega})/[L W L_\omega \Phi(E)]
\]

(9)

\[
dN_{\omega}/dt = - N_{\omega} r_s + [L W L_\omega R_{\omega}]/M' + (N_{\omega} r_s(E_{\omega}))/[\Phi(E)].
\]

(10)

where \( \eta \) is the internal quantum efficiency of the spontaneous radiation, \( m \) is the number of lasing modes, \( L \) and \( W \) are the length and width of the device, \( r_s \) is the photon lifetime in the lasing mode, and \( M' \) is the number of spontaneous modes. The number of modes per unit energy per unit volume is given by

\[
\Phi(E) = [\mu^2 E/[\pi^2 k^2 c^4]],
\]

(11)

where \( \mu \) is the refractive index. For simplicity one lasing mode is assumed \((m = 1)\) and since \( M' \) is typically quite large, the second term on the right side of eqn (10) is neglected. Now a steady state condition is assumed so that at threshold the two rate eqns (9) and (10) become:

\[
J_n = R_m c L |eL| \eta
\]

(12)

\[
r_s(E_{\omega}) = \Phi(E)/r_m
\]

(13)

These two equations contain two unknowns, \( r_s(E_{\omega}) \) and \( R_m \), which contain the unknown quasi-Fermi levels \( F_e \) and \( F_h \). \( F_e \) and \( F_h \) can be used to relate \( r_s(E_{\omega}) \) and \( R_m \) so that an expression for \( J_n \) can then be obtained.

(a) Strong electron-electron interaction (Fermi-Dirac distribution)

In the limit of strong electron-electron interaction eqns (1), (2) and (5) can be used in eqns (6) and (7) and result in

\[
r_s = - kT_e B g_e \ln A
\]

(14)

\[
r_p = -(kT_e B g_e \ln A)(1 - \exp (E' + F' - F_e))
\]

(15)

where

\[
A = ([\exp (F_1) + \exp (E')][\exp (F_1 + E') + 1])/(\exp (F_1 + E') + \exp (E') + 1)
\]

(16)

and where \( F' = F_e + E_{\omega}, \ E' = E - E_{\omega}, \ \text{and} \ a = F_e - F_h. \)

In order to calculate \( R_m \), \( \ln A \) is approximated in a piecewise linear fashion, giving

\[
\ln (A) = \beta E' \quad \text{for} \quad E' = 0
\]

(17a)

\[
= (E' - a)/2 \quad \text{for} \quad E' = a
\]

(17b)

\[
= E' - \ln (\gamma) \quad \text{for} \quad E' > a.
\]

(17c)

where

\[
\beta = (\exp (F_1))[\exp (F_1) + 1] - \exp (F_1)\] / [\exp (F_1) + 1]
\]

(18)

and

\[
\gamma = [1 + \exp (-F_1)]/[1 + \exp (F_1)].
\]

(19)

Typically \( F_1 = 0 \) and \( F_1 > 1 \) so that \( \beta = -1/2 \). Evaluation of eqn (6) yields

\[
R_m = (kT_e B g_e) (3a/4 + \exp (-a)[2a + 1 - \ln (\gamma)] - (2a^2)/8[1 - \exp (-a)])
\]

(20)

If the exponential term in eqn (20) dominates, we are left with

\[
R_m = (kT_e B g_e)[2a \exp (-a)].
\]

(21)

This gives the strongest temperature dependence of the threshold current. As can be seen from the following, the threshold current is almost independent of temperature if the \( a^2 \) term dominates. We now have to express \( r_m \) as a function of the quasi-Fermi levels, eliminate these terms, and solve for \( J_n \). This can easily be done numerically. However, an explicit solution, which contains all the essential features, can be obtained by assuming that \( E' = a/2 \), so that

\[
r_m(E_{\omega}) = (kT_e B g_e a^4/4).
\]

(22)

Relating eqns (12) and (13) through eqns (21) and (22) results in the following expression for \( J_n \):

\[
J_n = [(8eL_\omega \Phi(E))/\eta_{\omega}][(kT_e) \exp(-T^2/T_e)].
\]

(23)
Thus, in the limit of a strong electron-electron interaction, $J_{th}$ varies linearly (or weakly) with $T_c$ for large $T_c$. Note, however, that as mentioned earlier the carrier temperature, $T_c$, depends only weakly on the lattice temperature, $T$, for high densities of electrons scattering down in the quantum well by phonon emission. The result is a very weak dependence of $J_{th}$ on lattice temperature.

It is difficult to assess which of the two effects (the step-like density of states or the higher carrier temperature, $T_c$) reduces the temperature density of $J_{th}$ most. Comparing the result of eqn (23) with the calculations of Adams[14] for exponential band tails, we find a much weaker temperature dependence for the case of the step-like density of states even if $T_c = T$, the lattice temperature. The difference between eqn (23) and similar calculations for a parabolic density of states (3-D) is less pronounced. However, the parabolic density of states gives still a stronger temperature dependence.

The electron temperature $T_e$ is determined mainly by the power input per cm$^2$ which is of the order of 10$^7$ Watts/cm$^2$ for an active layer width of 100 A. Under these circumstances the electron temperature can be shown to be larger than about 200 K no matter how small the lattice temperature[10]. For lattice temperatures around 300 K electron temperatures of 350-400 K are typically expected. Accurate calculations are difficult to perform, however, due to many uncertainties concerning the phonon distribution function and scattering rates.

(b) Weak electron-electron interaction ($\Phi$-function distribution)

In the limit of a weak electron-electron interaction, eqns (1), (4) and (5) can be used in eqns (6) and (7) and yield

$$r_\omega(E') = kT_e g(E')[(\pi n L)^2/(m^* kT_e) - E']$$

(25)

$$r_\omega(E') = kT_e g(E')[(\pi n L)^2/(m^* kT_e) + 1 + \exp(\Delta E_e - m^* kT_e)]^{-1}$$

(26)

(Since $T_e$ has been assumed (after eqn 5) equal to $T_c$, for simplicity and to follow convention the symbol $T_e$ is used in the expressions of this section.)

The integrated spontaneous emission rate is then

$$R_\omega = kT_e g(E')[(\pi n L)^2/m^*]$$

$$\ln [1 + \exp(-F_e + \Delta E_e - m^* kT_e)](kT_e)^{-1}$$

(27)

The easiest case to evaluate is for small $E'_\omega$ so that

$$r_\omega(E'_\omega) = g(E'_\omega) [(\pi n L)^2/m^*]$$

(28)

Equations (12) and (13) may be relaxed in this limit by eqns (27) and (28) yielding for $|F'_\omega| < (\Delta E_e - m^* kT_e)/kT_e$
typical of a quantum-well heterostructure laser diode has been presented. In this analysis a step-like density of states has been used, and not the usual bulk-crystal parabolic density of states, which does not fit quantum-well heterostructures. Two limiting cases of weak and strong electron-electron interaction of the injected carriers have been considered. In both limits the threshold current density has been found to vary approximately linearly with carrier temperature, and to be only weakly dependent on lattice temperature which agrees with experiment. Data on single-quantum-well AlGaAs-GaAs heterostructure diodes ($L_s \sim 200\ \text{Å}$) have been presented showing that in the conventional expression $J_{th}(T) = J_{th}(0) \exp \left( \frac{e}{kT_0} \right)$ the temperature parameter $T_0$ can be as high as at least 437°C.

Acknowledgements—For assistance in portions of this work we wish to thank Yuri S. Moroz, R. T. Gladin, B. L. Marshall and B. L. Payne (Urbana), and J. E. Cooper, N. L. Lind, L. A. Moudy, T. J. Raab and J. J. J. Yang (Anaheim). We are particularly grateful to R. D. Dupuis for his contributions to the earlier phase of this work, and to J. J. Coleman and G. E. Stillman for helpful conversations. The work of the Illinois group has been supported by the national Science Foundation, primarily Grant DMR 76-17728 and to a lesser extent DMR 77-23999, and also Navy Contract N00014-79-C-0711. The work of the Rockwell group has been supported by the Office of Naval Research, Contract N00014-78-C-0768.

REFERENCES

Induced phonon-sideband laser operation of large-quantum-well Al$_x$Ga$_{1-x}$As-GaAs heterostructures ($L_z \sim 200\text{--}500$ Å)

J. J. Coleman and P. D. Dapkus

B. A. Vojak, W. D. Laidig, and N. Holonyak, Jr.
Department of Electrical Engineering and Materials Research Laboratory, University of Illinois at Urbana-Champaign. Urbana. Illinois 61801

K. Hess
Department of Electrical Engineering and Coordinated Science Laboratory, University of Illinois at Urbana-Champaign. Urbana. Illinois 61801

(Received 29 January 1980; accepted for publication 8 April 1980)

Data are presented on photopumped metalorganic chemically vapor-deposited Al$_x$Ga$_{1-x}$As-GaAs quantum-well heterostructures with active regions consisting of a large GaAs quantum well ($L_z \sim 200\text{--}500$ Å) coupled to a phonon generating array of seven small GaAs wells ($L_z \sim 50$ Å). Phonon-sideband laser operation below the confined-carrier transitions of the large GaAs quantum well(s) is induced by the large number of phonons generated in the smaller GaAs wells. The induced phonon-sideband laser operation (of a larger quantum well by an array of smaller wells) leads to a measurement of the energy difference between the first-state light- and heavy-hole energies of a 200-Å GaAs quantum well (4.9 meV) and directly to the GaAs LO-phonon energy $\hbar \omega_{10} = 41.0 - 4.9 = 36.1$ meV.

PACS numbers: 42.55.Px, 78.55. - m, 71.38. + i, 81.15 Gh

In contrast to the usual bulk crystal form of double-heterostructure (DH) lasers, quantum-well heterostructures (QWH's), as recently shown, are capable of laser operation on phonon sidebands. This is a consequence of the quasi-two-dimensional nature of quantum-well heterostructures and their steplike density of states. In previous work the possibility has been raised that stimulated phonon emission can occur in QWH lasers and should be most apparent in a multiple-well structure that forms a phonon resonator or cavity. To study these effects, in the present work we have constructed (and photopumped) two different metalorganic chemically vapor-deposited (MO-CVD) Al$_x$Ga$_{1-x}$As-GaAs multiple-quantum-well heterostructures, one with a single large GaAs well of size $L_z \sim 200$ Å coupled to a phonon generating array of seven small GaAs wells of size $L_z \sim 50$ Å and the second the same in form but with a single large well of size $L_z \sim 500$ Å. As shown below, in both heterostructures laser operation is observed one phonon below the lowest confined-particle states of the large wells, which is a much weaker or even nonexistent effect in a single-large-well heterostructure. The induced phonon-sideband laser operation of the larger wells leads to the result $\hbar \omega_{10} = 36.1$ meV, which is in good agreement with other measurements of $\hbar \omega_{10}$ (GaAs).

The Al$_x$Ga$_{1-x}$As-GaAs QWH's of interest here are grown by metalorganic chemical vapor deposition on GaAs substrates. Layer reproducibility is insured by electronically controlled gas flow rates and growth times. Following the growth of a GaAs buffer layer, a 1-μm-thick Al$_x$Ga$_{1-x}$As ($x = 0.35$) confining layer is grown. Next follows the multiple-quantum-well active region as described above with Al$_x$Ga$_{1-x}$As barrier layers of composition $x = 0.32$. The resulting effective electron density in the active region is shown in the inset of Fig. 1. Last is a 0.3-μm Al$_x$Ga$_{1-x}$As confining layer ($x = 0.35$) like the first. All layers are undoped ($n_e = n_h \leq 10^{15}$/cm$^3$); their sizes in all cases have been verified by SEM photomicrographs of shallow mesa etchings.

In previous work we have constructed (and photopumped) two different metalorganic chemically vapor-deposited (MO-CVD) Al$_x$Ga$_{1-x}$As-GaAs multiple-quantum-well heterostructures, one with a single large GaAs well of size $L_z \sim 200$ Å coupled to a phonon generating array of seven small GaAs wells of size $L_z \sim 50$ Å and the second the same in form but with a single large well of size $L_z \sim 500$ Å. As shown below, in both heterostructures laser operation is observed one phonon below the lowest confined-particle states of the large wells, which is a much weaker or even nonexistent effect in a single-large-well heterostructure. The induced phonon-sideband laser operation of the larger wells leads to the result $\hbar \omega_{10} = 36.1$ meV, which is in good agreement with other measurements of $\hbar \omega_{10}$ (GaAs).

The Al$_x$Ga$_{1-x}$As-GaAs QWH's of interest here are grown by metalorganic chemical vapor deposition on GaAs substrates. Layer reproducibility is insured by electronically controlled gas flow rates and growth times. Following the growth of a GaAs buffer layer, a 1-μm-thick Al$_x$Ga$_{1-x}$As ($x = 0.35$) confining layer is grown. Next follows the multiple-quantum-well active region as described above with Al$_x$Ga$_{1-x}$As barrier layers of composition $x = 0.32$. The resulting effective electron density in the active region is shown in the inset of Fig. 1. Last is a 0.3-μm Al$_x$Ga$_{1-x}$As confining layer ($x = 0.35$) like the first. All layers are undoped ($n_e = n_h \leq 10^{15}$/cm$^3$); their sizes in all cases have been verified by SEM photomicrographs of shallow mesa etchings.

\[ \text{FIG. 1. Emission spectra (77 K) of a photopumped multiple-quantum-well Al$_x$Ga$_{1-x}$As-GaAs heterostructure grown by MO-CVD.} \]

The rectangular sample is undoped ($n_e = n_h \leq 10^{15}$/cm$^3$) and contains an active region consisting of one 200-Å and seven 50-Å GaAs wells coupled by seven 50-Å Al$_x$Ga$_{1-x}$As barriers as illustrated in the inset. The confined-electron energy levels of the 200-Å GaAs well (left-hand side) and the 50-Å multilayer (right-hand side) and the 200-Å multilayer are shown in the inset. With increase in photopumping (see Fig. 1) from 200 W/cm$^2$ to 700 W/cm$^2$ the first transition begins to laser while simultaneously a spontaneous bump appears (b) one phonon below the first transition. With higher pump power (c) 1000 W/cm$^2$ the induced phonon-sideband transition 1-LO also laser.
low-angle cross sections,\textsuperscript{13} which agree with experimental observations (spectra) of the confined-particle transitions (identified on narrow samples 10–20 μm).\textsuperscript{3,6}

The MO-CVD Al\textsubscript{x}Ga\textsubscript{1−x}As-GaAs quantum-well heterostructures described above and shown in part in the inset of Fig. 1 are a design modification of the six-well (L ∼ 50 Å) quantum-well heterostructure corresponding to curve (b) of Fig. 1 in Ref. 2. These and related data,\textsuperscript{3,5} as well as recent analytical results and further data,\textsuperscript{14} show that the nonthermal phonon occupation number $N_{\text{ph}}$ can, in quantum-well heterostructures, be increased well above (≥ 500x, 77 K) the equilibrium value. This behavior has a profound effect in the present case because the large nonthermal phonon density generated in the closely coupled small wells can influence (stimulate) phonon generation and carrier scattering to lower energies in the larger coupled auxiliary (or “detector”) quantum well(s). For example, a highly excited large quantum well delivers recombination radiation from collected hot carriers from near $E_g$ to high above the band edge, as high as ~ 300 meV,\textsuperscript{2} but does not exhibit equally strong emission below the lowest confined-particle states (or $E_g$) unless assisted, as in the present work (Figs. 1–3).

The multiple-quantum-well heterostructures of interest here do not deliver appreciable recombination radiation higher than one phonon below the lowest states of the small wells, which in Figs. 1–3 is at $\lambda = 7750 \AA$ (or $E_g + 90$ meV). The coupled small wells cut off recombination from higher in the larger single 200-Å well (Figs. 1 and 2) or single 500-Å well (Fig. 3). Photogenerated higher-energy carriers are collected (from the confining layers) in the active region and tunnel into the small-well section; scatter downward, generating phonons in an efficient layered structure (seven coupled 50-Å GaAs wells) that can act as a phonon cavity\textsuperscript{3,8} and then at much lower energy tunnel back into the big well for further scattering and recombination. The phonons generated in the small-well section assist the further downward scattering in the single large well, and lead to the unique form of low-energy laser operation shown at $\lambda = 8343 \AA$ in Figs. 1 and 2 and $\lambda = 8400 \AA$ in Fig. 3.

The data of Fig. 1 are unique. The high-level spontaneous emission intensity, obtained by photopumping across part of the width of a rectangular sample,\textsuperscript{1,2,3,6} is given by curve (a). When the photopumping is slowly increased from
A single laser mode emerges abruptly on the first electron-to-light-hole \( (n' = 1) \) transition and simultaneously a prominent bump appears on the (b) curve one phonon below the first electron-to-heavy-hole \( (n = 1) \) transition \( (E_r - \hbar \omega_{11}) \). At still higher pumping \( (c) \) the \( n' = 1 \) mode still predominates, and the transition at \( E_r - \hbar \omega_{11} \) narrows into stimulated emission. The excitation can be adjusted on the sample slightly, giving the data of Fig. 2. The \( n' = 1 \) mode is still identifiable and an LO phonon below \( n' = 1 \) and below \( n = 1 \) two bumps appear due to rapid light-hole-to-heavy-hole relaxation \( (\sim 10^{-12} \text{s}) \). We can expand this portion of the spectrum (inset) and measure, accurately, as shown, the \( 1' - 1 \) spacing and in turn the LO phonon energy, which is \( \hbar \omega_{11} = 41.0 - 4.9 = 36.1 \text{ meV} \).

It is clear that if the data and ideas above are correct, by merely increasing the size of the larger well we should be able to shift the lower confined-particle transitions (to still lower energy) and with them the induced phonon-sideband emission lines. This is what is observed in Fig. 3 for a larger well of size \( L_z = 500 \text{ A} \) at a fairly high level just above the threshold for stimulated emission \( (\text{as} 1.2 \times 10^4 \text{ W/cm}^2, \text{cw}) \) length-to-width \( (l = 50 \text{ mm}) \) laser modes appear abruptly on \( n' = 1' \) (or \( 1' - \text{LO} \)). Then at higher pulsed excitation \( (\text{as} b), 5 \times 10^4 \text{ W/cm}^2 \) further end-to-end modes appear at \( 1' - \text{LO}, 2' - \text{LO}, 2' - \text{LO} \), which is quite remarkable, and still one more set of modes appears (edge to edge, \( w = 59 \text{ mm} \)) at \( \lambda = 8260 \text{ A} \), which is in the range one phonon below transitions 3 and 3'. These transitions \( (3, 3') \) have a higher density of states and higher oscillator strength, which could explain their involvement in edge-to-edge laser operation.

Note that the laser emission on the phonon sidebands in \( b \) of Fig. 3 is the dominant recombination radiation, i.e., is not a weak effect if the sample is of sufficient size. If we reduce the sample width sufficiently \( (w = 23 \text{ mm}) \) and thus increase the cavity end losses, as in Fig. 3(c), the main laser operation, on widely spaced edge-to-edge modes, moves up to the region of the lowest confined-particle transitions and the band edge, which is nearby \( (2.4 \text{ meV}) \). Even in this case weak end-to-end \( (l = 211 \text{ mm}) \) laser modes are observed in the region \( 1' - \text{LO}, 1' - \text{LO} \).

We interpret the unique location and manner of turn-on of the spectral bump and emission line marked by the arrow in Fig. 1 and the various LO arrows on Fig. 3(b) as a sign of stimulated phonon emission. In addition, we have been able to measure the first-state light-hole-heavy-hole quantum-well energy separation and measure directly the LO phonon energy in GaAs \( (\hbar \omega_{11} = 36.1 \text{ meV}) \).

We wish to thank Yuri S. Moroz, R. T. Gladin, B. L. Marhsall, and B. L. Payne (Urbana) for technical assistance. The work of the Illinois group has been supported by NSF Grants DMR 79-09991 and DMR 77-23999 and Navy Contract N000 14-79-C-0768; the work of the Rockwell group has been partially supported by the Office of Naval Research, Contract N000-14-78-C-0711.

\[ ^1 \text{N. Holonyak, Jr., R. M. Kolbas, W. D. Ladig, M. Altarelli, R. D. Dupuis, and P. D. Dapkus, Appl. Phys. Lett. 34, 502 (1979).} \]
\[ ^3 \text{B. A. Vojak, N. Holonyak, Jr., R. Chin, E. A. Rezek, R. D. Dupuis, and P. D. Dapkus, J. Appl. Phys. 50, 5835 (1979).} \]
\[ ^4 \text{E. A. Rezek, R. Chin, N. Holonyak, Jr., S. W. Kirchoefer, and R. M. Kolbas, J. Electron. Mater. 9, 1 (1980).} \]
\[ ^6 \text{N. Holonyak, Jr., R. M. Kolbas, R. D. Dupuis, and P. D. Dapkus, IEEE J. Quantum Electron. QE-16, 170 (1980).} \]
\[ ^7 \text{N. Holonyak, Jr., R. M. Kolbas, E. A. Rezek, R. Chin, R. D. Dupuis, and P. D. Dapkus, J. Appl. Phys. 49, 5392 (1978).} \]
\[ ^8 \text{K. Hess, Appl. Phys. Lett. 25, 464 (1979).} \]
\[ ^9 \text{A. Moorsadian and G. Wright, Solid State Commun. 4, 431 (1966).} \]
\[ ^10 \text{H. M. Manasevit, J. Electrochem. Soc. 118, 647 (1971).} \]
\[ ^12 \text{R. D. Dupuis and P. D. Dapkus, IEEE J. Quantum Electron. QE-18, 128 (1970).} \]
\[ ^13 \text{N. Holonyak, Jr., B. A. Vojak, R. M. Kolbas, R. D. DuPuis, and P. D. Dapkus, Solid State Electron. 22, 431 (1979). Note that this measuring technique has been further refined with Dekia Sloan Instruments angle and SEM layer measurements and now gives good size estimates.} \]
\[ ^14 \text{K. Hess, N. Holonyak, Jr., W. D. Ladig, B. A. Vojak, J. J. Coleman, and P. D. Dapkus, Solid State Commun. (to be published).} \]
Hot electrons in layered semiconductors

The size of semiconductor devices has decreased so much that classical treatments of semiconductor physics become invalid and effects involving supra-thermal electrons take on a new importance.

Karl Hess and Nick Holonyak, Jr

As electronic systems—and especially computers—are used more and more widely in almost all areas of endeavor and daily life, the semiconductor technology on which they are based is being pushed to ever larger-scale integration and ever greater miniaturization. As the devices get smaller, and smaller, new problems (and maybe new opportunities) appear.¹

One consequence of the reduction in size is that the fields accelerating electrons and holes through the crystal become very large, so that the carriers acquire large kinetic energies. The equations of motion for an energetic electron can be appreciably different from Newton's laws; its (inertial) mass can, for example, appear to be infinite or even negative. This has nothing to do with relativistic effects but is due to Bragg reflection. The non-linearity of the equation of motion is illustrated in figure 1, which shows lines of equal energy in momentum space (k-space) for the semiconductor gallium arsenide.² For a free particle, these lines would be circles, as they are near the origin in figure 1, because the energy depends on only the magnitude of the momentum. The complicated shapes of the curves for large k indicates that the relation between energy and momentum is anisotropic and not quadratic. Electrons then do not necessarily move in the direction of the electric field and their average speed is not simply proportional to the field strength; that is, Ohm's law breaks down. We shall discuss this point more extensively later.

To illustrate the reduction in size that has accompanied the progress of semiconductor technology, we show in figure 2 the original point-contact transistor and a modern layered quantum-well heterostructure. (We should point out, though, that the point-contact transistor was a much smaller device than the junction transistors that were subsequently most widely used in practical devices.)

As we mentioned, the electric fields in small devices can become very large. If we assume that operating voltages of semiconductor devices are around 5 V, then the maximum electric fields in a typical device of twenty years ago was on the order of 10–100 V/cm. In a present-day integrated circuit the average fields are 10² V/cm and maximum fields are an order of magnitude larger. At such field strengths silicon and germanium become non-Ohmic at room temperature.³ Fields on the order of 10⁵ V/cm are encountered between neighboring gates of charge-coupled devices and in quantum-well layered devices. Such large fields may also be approached in the very-large-scale integrated circuits that are now being developed.

At fields larger than 1000 volts/cm the charge carriers in a semiconductor are accelerated far above their thermal-equilibrium energy (given by the lattice temperature). Under these circumstances so-called “hot-electron effects” become important and many of the familiar concepts of semiconductor physics lose their validity. In this article we will discuss some of the effects that will be important in future very-large-scale integrated circuits and in optoelectronic devices.

Hot electrons

As electrons move through the crystall lattice, they interact both with each other and with the lattice. In electronic devices, the applied electric field supplies energy to the electrons. If electron-electron collisions randomize the carrier energy, one can define a temperature for the electrons even for very high fields. This temperature \( T_e \) is always higher than the temperature of the crystal lattice \( T_L \). The difference between \( T_e \) and \( T_L \) depends strongly on the electric field (actually on the square of the field because reversal of the field must not lead to negative temperatures) and on the details of how the electrons lose their energy. In all practical cases the electrons lose their energy to lattice vibrations. We thus have a picture of a highly mobile fluid at high temperature (the “electron gas”) moving through the cooler crystal lattice and losing energy to it.

We know that conducting wires begin to slow if too much energy is transferred from the electron gas to the crystal lattice. We would like to emphasize, however, that even if the lattice remains cold (a situation that often can be arranged), the temperature of the electrons can be exceedingly high and cannot be controlled by any cooling mechanism (other than the slow heat loss to the lattice). A typical example would be a piece of silicon, let us say, to which an electric field of 2×10⁶ V/cm is applied; the electron temperature rises to 1000 K no matter what the
Surfaces of equal energy in the Brillouin zone of gallium arsenide calculated by the empirical pseudopotential method. (The Brillouin zone is the hexagonal area; the figure shows a somewhat extended zone.) Ohm’s Law holds only for electrons at the lowest energy (dark gray). The carrier energy increases from gray (center) to white to red to dark red in steps of 0.5 eV.

Figure 1

Surfaces of equal energy in the Brillouin zone of gallium arsenide zone. Ohm’s Law holds only for electrons at the lowest energy (dark gray). The carrier energy increases from gray (center) to white to red to dark red in steps of 0.5 eV.

Figure 1

temperature of the surrounding medium or heat sink attached to the sample. One consequence of this rise in temperature is that the conductivity drops because of the Bragg reflection mentioned earlier and because hot electrons can excite more lattice vibrations than cooler (lower-energy) electrons. The electrons are thus less mobile, being scattered more often. The conductivity therefore depends on the field strength and Ohm’s law is not valid at these high fields. It is worth mentioning that the heating of the electron gas (not the lattice) is very fast. Typically, the time constant is $10^{-12}$ sec.6

Keeping the electron gas in equilibrium with the lattice would mean using smaller electric fields. As the devices get smaller, the voltages would thus also have to get smaller. However, for various reasons it is unlikely that the supply voltages applied to semiconductor devices can be reduced below one volt. One reason is the variation in threshold voltages of the component devices. Another is that the built-in voltages (or potentials) of semiconductor devices are of the order of the semiconductor energy gap, which is a property of the crystal, and cannot be scaled down. We can therefore expect that future semiconductor devices will inevitably involve hot-electron effects in their operation. It is not clear, however, which of the various hot-electron effects will be most important.

Current device concepts that might involve hot-electron effects are carrier (electron or hole) drift, diffusion, generation-recombination, and thermionic emission over potential barriers.3

Clearly it will not be possible to cover all possibilities in a short article. We therefore concentrate, as examples, on effects specific to hot electrons in potential wells. The reason for this choice is that with shrinking crystal size the charge carriers become increasingly confined to narrow potential wells as defined by the size of the components.

Layered devices

To illustrate the effects one expects with narrow potential wells and high electric fields, consider the layered structure shown in figure 2. The general properties of such a structure are sketched in figure 3. The layers could be InP and InGaPAs (as in the sample shown in figure 2) or (as in figure 3) GaAs and Al, Ga, As; these layers have now been produced by several different methods, including molecular-beam epitaxy, metal-organic chemical vapor deposition and liquid-phase epitaxy. The layers in these structures range from $10^{-5}$ to $10^{-3}$ cm in thickness. Such structures are in many ways prototypes of a variety of devices including field-effect transistors and charge-coupled devices.

On the small scale of these layers, charge-neutrality is not preserved because electrons move from one layer into another without creating substantial electric fields, that is, they leave regions of high potential energy and move into potential minima.

In the sandwich shown in figure 3, Al, Ga, As-GaAs-Al, Ga, As, the properties of the electrons change substantially in the middle layer:

- Because of the constraining AlGaAs layers the electrons are not free to move perpendicular to the layers and hence form a two-dimensional gas. As a consequence, their minimum energy (remember the famous quantum-mechanical problem of a particle in a box) lies above the GaAs conduction band edge ($E_c$). We refer to this effect as “size quantization.”

- The electrons in their motion are scattered either by lattice vibrations (phonons) or by various impurity centers, which can be small in number in the GaAs. The “remote” impurities (electron donors or acceptors) in the layers of Al, Ga, As do not influence the electron motion. As a consequence, the electrons in the GaAs layer are more mobile as compared to bulk material if the donors are mainly in the Al, Ga, As layers. This notion was proposed originally by Raphael Tsu and Leo Esaki (IBM) and recently demonstrated by Raymond Dingle, Arthur Gossard, Horst Stormer and William Wiegmann (Bell Labs).1

Less well known than the impurity-scattering case above is the fact that the scattering of electrons by lattice
the interface mobility of electrons and hence the device speed.

Let us return to the layers of GaAs and AlGaAs (figure 3) and assume the electrons are in the middle layer (GaAs) before we apply an electric field parallel to the interfaces. As long as the applied electric field is small, the electrons will stay in the GaAs. For large electric fields, however, the electrons will be heated, and move up in energy, and finally when their energy approaches the band edges in the surrounding AlGaAs, they can transfer out into the adjacent layers. It is clear that this effect has a close analogy to thermionic electron emission out of glowing wires, as in a vacuum tube, or to the momentum-space electron transfer that occurs in the Gunn effect, which is the basis for useful microwave devices. A Monte Carlo simulation of the electron trajectory for carrier transport in a thin (400 Å) GaAs layer is shown in figure 4. For an undercritical field, the electron stays in the GaAs well. For a field above a critical threshold, the electron can transfer out into the surrounding AlGaAs. A variety of effects perhaps can be created using the mechanism of hot-electron transport out of thin layers.\(^8\) Some of these have just recently been verified experimentally.

**Very-large-scale integration**

At this point let us shift to more established ground and consider the hot-electron effects that occur in very-large-scale integrated circuits. Tak H. Ning at IBM has shown\(^9\) that in the metal-oxide-semiconductor system (so important in present-day integrated circuits) electrons can be emitted from silicon into the silicon dioxide over potential barriers that are quite large. In the silicon dioxide the electrons are finally trapped and give rise to unwelcome changes in the interface potential, causing instabilities in the device performance. These effects occur on long time scales, but are important in general.

An even more pronounced example is the so-called "buried-channel structure," which is diagrammed in figure 5. This structure was conceived to avoid trapping of electrons at the silicon-silicon-dioxide interface. The crucial feature is that of an ion-implanted layer which creates the potential-energy profile shown in the lower part of the figure. As in the case of the GaAs-AlGaAs layers discussed above, the electrons are at minimum potential energy (between \(x_1\) and \(x_2\)) far away from the silicon-silicon-dioxide interface. Structures such as this are used for charge-coupled devices and metal-oxide-semiconductor transistors. If we now shrink the device, we obtain much higher electric fields, which,

---

**Figure 2**

**Figure 1**

**Figure 1A**

**Figure 1B**

Evolution of the size of electronic devices. (a) Original transistor patent of John Bardeen and Walter Brattain: The germanium crystal is about 0.1-0.5 cm in size, while the spacing between the emitter and the collector (labeled 5 and 6) is considerably smaller. (b) Layered structure: a quantum-well heterostructure laser, of InGaPAs quaternary compounds grown by liquid-phase epitaxy. To illustrate the layer sizes, leukemia viruses of about 500 to 1000 Å diameter are shown superimposed on the crystal layers.

**References**


when the device is in operation, accelerate and heat the electrons. The consequence is that electrons can be thermionically emitted to the interface again as occurred for the GaAs-AlGaAs layers. The device then loses its advantage of being a buried-channel device; we have reached a limit in how much we can reduce the size of the device.

Of course, high electric fields also influence the electron drift within the potential wells themselves, even before thermionic emission occurs. In metal-oxide-semiconductor devices, therefore, the drift velocity of electrons always saturates with increasing electric field. The reason for this is the enhanced scattering of hot electrons by lattice vibrations, as has long been known.

The mechanisms described above have drastic effects on device properties. We should also expect a dramatic influence of high fields on carrier diffusion. Steep concentration gradients and high electric fields totally invalidate the basic concept of particle diffusion as described by the classic Einstein relation, \( D = \frac{\mu kT}{e} \). Preliminary investigations show that the usual diffusion constant, \( D \), has to be replaced by a rather complex expression even if the device is large enough that the electron is not able to traverse it without collisions, which clearly violates the basic ideas about diffusion.\(^\text{11}\) This brings us to the limiting size of small devices: If we shrink the size still further, how long do we have enough electrons to apply familiar statistical concepts, and what is the limit of size for ballistic transport of charge carriers? That is, where does the semiconductor become like a vacuum for the electron? The answers to these questions are urgently needed; a number of commercial semiconductor products touch these borders already, and clearly many more will in the near future.

Before turning to opto-electronic layered-structure devices, specifically quantum-well lasers, which so clearly show a strong deviation from bulk crystal behavior, we summarize in the box on the right the deviations from well-known physics and engineering principles that we expect for small devices. We cannot give a comprehensive description of all the effects we list. We have discussed quantization, velocity saturation, and hot-electron emission. The overshoot effects listed in the box are connected with energy and momentum relaxation by collisions. Some of the effects (such as the \( \text{Franz-Keldysh effect} \)) have been known for a long time but up to now have been unimportant in device applications. The rest are connected with the unusual boundary conditions (interfaces) in small devices and layers, and with the small number of charge carriers and impurities in the extremely small volume.\(^\text{1}\)

### Opto-electronics

So far we have discussed hot-electron effects that are driven or engendered by an applied electric field, as in a transistor or Gunn-effect oscillator. As a prototype for various forms of semiconductor lasers, and perhaps other optoelectronic or integrated-optics devices, let us assume that the-middle

---

**Effects expected for small devices**

- **Drift**
  - Deviations from Ohm's Law
  - Saturation of current
  - Velocity overshoot
  - Ballistic transport
  - Mobility increased or decreased by size effects (remote point charges, phonons)
  - Scattering—high electric fields
  - Generation of high phonon intensities

- **Diffusion**
  - Hot-electron diffusion and invalidation of the Einstein relation
  - Enhancement of diffusion constant by high electric fields
  - Anisotropy of diffusion
  - Diffusion and reduced dimensionality
  - Diffusion overshoot

- **Carrier generation and recombination**
  - Poole-Frenkel enhancement of emission out of potential wells (traps)
  - Hot electron "thermionic" emission
  - Effects of hot electrons on the \( \text{Franz-Keldysh effect} \)
  - Impact ionization (inverse Auger process) can determine ultimate limits of speed, and so forth.

- **Generation-recombination noise for non-stationary case (Langevin)**

- **Size effects**
  - Size quantization (two-dimensional, one-dimensional electrons)
  - Quantum resonances
  - Interfaces, surfaces, metal boundaries and effects of these boundaries on important semiconductor parameters.
  - Image force (metal boundaries)
  - Non-ideal interfaces
  - Contacts as boundaries
  - Density-size relations
  - Steep concentration gradients and high electric fields. (See diffusion)
  - Alloy effects (atom disorder)
  - Low-level radiation effects (\( \alpha \)-particles from package)
  - Interconnection problems (sheet resistance)

---

**Layered structure, consisting of gallium arsenide and aluminum gallium arsenide.** The graphs show the impurity doping concentration, the carrier mobility and the energy of the edge of the conduction band of this modulation-doped structure. Figure 3.

**Electron motion, computed by a Monte Carlo simulation, in a potential well formed by a gallium arsenide layer.** The wells are broad enough (400 \( \AA \)) that they show no effects due to size quantization. On the left the field strength is 2 kV/cm, below the threshold for jumping out of the well; on the right the field is 8 kV/cm. Figure 4.
layer of GaAs in figure 3 is 200 Å thick and that the Al$_x$Ga$_{1-x}$As layers on either side are 0.5-1 micron thick. If we put the structure in contact with a good heat sink and photopump it with an intense light source, electrons and holes are generated in the Al$_x$Ga$_{1-x}$As layers and will be collected in (a very short time) in the GaAs potential well. Relative to the bottom of the GaAs well, however, these electrons are "hot," that is, they are high above the GaAs band edge $E_c$. In energy and can either scatter downward to the bottom of the GaAs well, releasing lattice vibrations (phonons) in the process, or, while still hot and high in the well, they can recombine with holes, releasing high-energy photons (red, not the usual infrared of bulk GaAs). This is a remarkable effect: a crystal system that normally (in bulk) emits infrared light, when made into a quantum well, emits (via the recombination of hot electrons and holes) true red light.$^{12-14}$ This is shown in figure 6 by the laser emission near 7000 Å.

The hot-carrier red-light emission from GaAs shown in figure 6 was first observed by Robert Kolbas and Holonyak$^{12}$ on quantum-well crystals first grown by their coworkers at Rockwell International, Russell Dupuis and Daniel Dapkus and, later, James J Coleman. We should mention that the quantum-well structure that emits the red light (as well as the longer-wavelength infrared laser light) of figure 6 can be constructed by putting doped $p$-type material on one side of the GaAs quantum-well and $n$-type on the other side; it then operates as a unique form of injection laser: a hot-carrier quantum-well semiconductor laser.

It is also possible to insert, or couple together, more than one quantum well in the center of the structure as the layered structure of figure 2 shows. In that case, the hot-carrier collection and the downward scattering into the quantum wells can be much more efficient. If the number of these quantum wells is not too great and the wells are not too thick, say six wells, each 50 Å thick, one can observe still another important effect at sufficient excitation (photopumping or current excitation): The hot carriers scatter down towards the bottom of the quantum wells and, instead of recombining at the first (lowest) quantum states of the coupled GaAs wells, the carriers will scatter down even further and produce laser emission on a phonon sideband.

Just as the collection and the scattering of hot carriers to lower energy in a layered structure is improved when more than one quantum well is employed, carrier scattering to lower energies in a single potential well is constrained—and, in fact, makes possible the hot-carrier electron-hole recombination observed$^{12,18}$ over the unusually large wavelength range of figure 6. If the rather large (200 Å thick) well that produced this spectrum is reduced in thickness to much under 100 Å, then the size constraint does not permit carriers to scatter down to the lower quantum states before recombination occurs. When a single potential well becomes as small as 50 Å, the highly mobile electrons can travel all the way across the potential well before colliding with the lattice. For excessively thin layers, then, the hot electrons tend to travel right across the very narrow well instead of scattering, losing energy, and descending into the well.

If these ideas and observations have much validity, it should be possible to verify them by still other means. Hot carriers lose energy by collisions with the crystal lattice, thereby converting some of their energy to increased lattice vibrations, or, equivalently, increased phonon density. The process is strong when the coupling between the charge carriers and the lattice vibrations is strong. The electron-phonon coupling can be screened by introducing a large background of free carriers into the crystal, such as a large number (10$^{19}$cm$^{-3}$ or more) of positive holes—which can be introduced by diffusing zinc atoms to serve as acceptors into the layered structure. The screening is such a powerful effect that when carried out on the sample that produced figure 6, the weakening of the electron-phonon interaction almost cuts off the carrier scattering into the well: the hot carriers no longer scatter into the (rather large) quantum well, and the laser spectrum vanishes.$^{15}$

We have to construct a much bigger active region to be able to see that the zinc doping merely screens the elec-
Comparison of laser spectra of (a) an undoped and (b) a Zinc-doped (hole density $10^{14}$ cm$^{-3}$) layered heterostructure consisting of six $120$-Å GaAs quantum wells coupled by five $120$-Å AlGaAs barriers. In (a) the photo-generated hot carriers thermalize to low energy while with the zinc impurity, in (b), the electron-phonon interaction is screened, so the carriers remain hotter and recombine at higher energy ($100$ meV). Figure 7.
	ron-phonon interaction and does not in fact damage the layered structure, and thus “kill” the light emission of the GaAs quantum wells. The screening effect of the doping is seen in figure 7. The theory that produced these graphs consists of six layers ($120$ Å thick) of GaAs separated by five equally thick layers of AlGaAs. The top spectrum shows the laser emission from the undoped sample one phonon below the lowest quantum states (1'). When zinc doping is introduced into the sample (generating, as we said, a large background of holes), the photogenerated hot carriers cannot thermalize to low an energy before recombination (because of screening and a weaker electron-phonon coupling), and the laser operation (curve b) shifts up in energy by $100$ meV to the region of the second quantum states (2') of the coupled quantum wells. That is, the high-energy laser operation at $7655$ Å of curve b involves the recombination of carriers that are hotter than those leading to the laser operation ($8180$ Å) at the lower energy of curve a.

It is worth mentioning that the results of figure 7 are in excellent agreement with the hot-electron effects mentioned earlier. The quantum-well laser operation occurring at $7655$ Å in curve b of figure 7 corresponds to an electron temperature of about $1330$ K compared to a lattice temperature of about $77$ K (the copper heat sink for the crystal is immersed in liquid nitrogen). In essence, the impurity screening has switched off some of the carrier energy loss to the lattice (to phonons), and, as a consequence, more of the input energy emerges from the crystal as higher-energy recombination radiation (crystal laser output).

Small devices

Although the ideas and examples presented here concerning hot-electron effects in semiconductors are not exhaustive, they are representative and show clearly that newer semiconductor devices, as well as a higher level of integrated circuit development and smaller sizes, will inevitably make hot-carrier effects more and more important. Making semiconductor elements smaller and closer together to increase the number of active elements per square centimeter or per chip, is not a matter of just finding methods of reducing device size and generating a microscopic system of element interconnections. New physical effects and processes are necessary.

The increased power densities involved in small-device operation makes higher-order processes important. For example, we mentioned above in some detail the phonon sidebands that appear in quantum-well heterojunction lasers. It is clear, however, that high phonon densities are also generated:

- during material processing such as laser annealing
- by the exceedingly high local current densities possible in VLSI elements
- in research such as picosecond spectroscopy.

The simple statement in solid-state textbooks that indirect optical processes (involving phonons) are unimportant ceases to be true even in the case of direct semiconductors.

Another aspect of the sample is connected with the unusual boundary conditions in small structures. The cyclic (Born-von Karman) boundary conditions, which are so convenient in solid-state theory, are inappropriate for quantum-well heterostructures and for very small devices. Instead of finding a "repeated crystal" after a large number of atoms, the electron can, as we know, transfer out of the silicon into the silicon dioxide and thereby limit the functioning lifetime of semiconductor devices. This process involves electron energies of about $3$ eV above the conduction-band edge. The interesting question therefore arises whether this emission process can be avoided by using supply voltages lower than $3$ volts or by using band-structure effects such as Bragg reflection. This question is also relevant for the possibility of high-speed, low-temperature silicon circuits but is too complicated for us to discuss here in detail.

The effect of hot-electron emission can possess positive aspects, as it can clearly be used to construct ultra-fast electronic switches. The issue of boundary conditions and size effects also opens fascinating possibilities for optoelectronic devices, which are illustrated, for example, by the red-light emission of gallium arsenide.

Small integrated semiconductor devices already have had a strong impact on our daily lives; the impact promises to continue and, in fact, increase in scope. This will in turn further stimulate research in the field of "ultra-small electronics."

We are indebted to John Bardeen and Charles B. Duke for helpful comments, and to the NSF, the Navy, and the Army for support.

References

11. See the papers of D. K. Ferry and J. R. Barker, in reference 1.