December 17, 1991

Defence Technical Information Center
Bldg 5, Cameron Station
Alexandria, VA 22314

Re: Grant No. N00014-89-J-2038

Dear Sirs,

Please find attached my “final report” for Grant No. N00014-89-J-2038. Copies of the final report have been sent off to the Scientific Officer at Naval Research Laboratory and the Director at NRL.

Yours sincerely,

L. R. Ram-Mohan
Professor of Physics & Electrical Engineering

cc: ONR Resident Representative
MIT, Cambridge, MA 02139
The theoretical development of the transfer matrix method (TMM) by me has provided a compact and efficient algorithm for the band structure of superlattices.

- It has been the mainstay in the interpretation of experimental data on magneto-optics and magneto-transport in zero-gap superlattices of HgTe/CdTe at three institutions: NRL, Notre Dame, and MIT. A complete picture has emerged which is able to explain the observed magneto-optical spectra by including contributions throughout the entire superlattice Brillouin zone.

- The analysis of piezomodulation studies at Purdue was also performed using this method. Parabolic well heterostructures were studied using piezomodulation which revealed a rich spectrum of transitions all the way from the spin-orbit split-off band quantum well levels to the conduction band levels. The theory work was done at WPI.

- Theoretical investigations at WPI of the optical nonlinearity $\chi^{(3)}$ in superlattices of GaAs/AlGaAs have been based on the TMM. We have investigated in a systematic manner the issue of determining the optimal widths for the wells and barriers in order to increase the optical nonlinearity.
Work was done at NRL on investigating effects of lateral confinement in very narrow-gap superlattices, using the TMM algorithm to induce the lateral confinement through the use of a magnetic field. This has led to predictions of an energy level spectrum in such materials which displays unusual features in energy level spacing and level-filling effects which suggest that resistance quantization is not an integral multiple of the fundamental factor of $2e/h$.

More recent work at the NRL has predicted a magnetic field induced transition from semiconducting to semimetallic behaviour at zero temperature in narrow-gap semiconductors. Again, this work was made feasible through the TMM.

As promised in the proposal, the ability to study superlattice structures with arbitrary growth direction was implemented in the TMM algorithm. Calculations on type I and II superlattices with arbitrary growth direction, with built-in strain, and in the presence of external magnetic field, can now proceed ahead.

At present the TMM is capable of including effects of (i) a magnetic field applied perpendicular to the layers, (ii) strain in the layers for any III-V or II-VI layered quantum heterostructures. The following items need to be studied.

- **Modulation doping and a selfconsistent calculation of band bending in superlattices and quantum wells**
  So far I have studied the issues and problems in a one-band model. The experience suggests that I should use the finite element method for this problem (see below). This is being investigated at present by me.

- **Quantum Wells**
  The 8-band TMM has been set up for superlattices only. It is important to implement the programs for quantum wells as well. **Over the past 3 months I have been able to (i) clarify why the TMM algorithm has some instabilities which create vexing problems for calculations with it (this is due to the presence of spurious states, which can be identified and eliminated); (ii) develop the theoretical model for the calculation of energy levels in quantum wells. These two developments in the theory of the TMM suggest that I should review the programs and up-date them in the light of the accumulated experience over the past 3 years with the TMM.**

- Work is in progress to extend its applicability to modulation doping and to electric field effects.

The student supported by NRL has also been working on the issues of developing tight-binding models and algorithms for the investigation of (i) band structures of bulk III-V and II-VI semiconductors with special emphasis on evaluation of deformation potential constants at the band-edges and for intervalley scattering; (ii) the band structure of superlattices and quantum wells in very narrow layers (short-period superlattices, $\delta$-doping effects, etc); (iii) superlattice band structures for materials with energy minima away from the Brillouin zone center, such as PbTe-PbSnTe superlattices, etc.

The list of publications is attached.
PUBLICATIONS DURING 1989-1991

The Transfer matrix method and its applications


4. "Room Temperature Magnetooabsorption in HgTe/Cd_{0.85}Hg_{0.15}Te Superlattices"; K. H. Yoo, R. L. Aggarwal, L. R. Ram-Mohan, and O. K. Wu, *J. Vac. Sci. Technol.* A 8, 1194-1199 (1990).


The Finite Element Method and its Applications

