At the present, Duke favors a model in which unconnected on GaAs system and this project has been turned over to Kahn. Duke et al have suggested this problem to the importance of the metal-GaAs interaction. Skeath and Goddard have proposed a completely ordered overlayer. Skeath and Harrison on the basis of bonding considerations. Zunger and W. Goddard et al for somewhat different reasons.

Mechanism of Oxygen Chemisorption on GaAs

For both fundamental and practical reasons, we consider it very important to obtain a definitive understanding of the chemisorbed phase of oxygen on GaAs. This is the phase obtained with unexcited oxygen characterized by a completely resolved 2.9 eV As-3d shift and an asymmetric broadening of the 0.7 eV. These shifts correspond to those obtained by Goddard's group (1) for oxygen attached to a surface As without breaking any back bonds. This was also our original suggestion for the chemisorbed oxygen. Problems with this model involved the dynamics of the break-up of the O2 molecule.

Goddard et al (2) and Mark et al (3) suggested that this was done at defect sites with the oxygen uptake spreading outward from these sites. Our recent work shows that this is not the case. In addition, we have given definitive evidence that the model of Brundle et al (4), which assumes that there is no chemisorbed state -- only clusters of AsO and GaO isotopes is not correct. Finally, we have new evidence for a second major adsorption site which, in addition to an oxygen bonded to an As, there is another bonding between that As and a next nearest Ga (5).

Essential to arriving at these conclusions have been extensive experiments. These experiments have included the development of new valence band spectroscopy in which very low concentrations of adsorbed oxygen can be detected (0.001 monolayer) (6), thermal desorption, studies of the valence band of Ga-3d and As-3d, and photocatalytic reaction of adsorbed oxygen on disordered sputtered Ga-rich GaAs (110) surfaces. This work is part of the Ph.D. thesis of C.Y. Su, and will be published soon.

Mechanism of Adsorption of Column III and V Elements on GaAs

We have found that the column III elements do not bond "atomically", as predicted by all theorists who had considered this problem (6-9). This now appears to be accepted. This leaves open the very important question of how the metal is bonded to the surface. Recent theoretical estimates of the binding energy of column III elements to the surface by A. Zunger and W. Goddard et al for somewhat different models give a relatively small value of about 0.5 eV. From our work and the available calculations of column III molecules in two-dimensional islands on the surface, it is clear that metal-metal interactions are comparable to the importance of the metal-GaAs interaction.

It is clear that Sb (column V) forms an ordered overlayer. Skeath and Goddard have proposed detailed models (10). We intend to use angle-resolved photoemission to distinguish between these.

May 1981 work on column III and V elements overlayers has been carried out by our group in collaboration with A. Kahn of Princeton University. It has been definitively established that Drillon's report of ordered Al on GaAs at room temperature was incorrect (11). Additional studies have been made of the Sb on GaAs system, and this project has been turned over to Kahn. Duke et al are analyzing Kahn's data. At the present, Duke favors a model in which unconnected Sb molecules are adsorbed on Ga sites. This model has been considered and discarded by Skeath and Harrison on the basis of bonding considerations. In the future, angle-resolved photoemission will be used to help distinguish between this model and others.
Comparison of Our Work with that of Others

In general, very satisfactory agreement is obtained between our work and that of others. Previous disagreement between our work and that of Brillson et al. (12) had caused some confusion; this has recently been resolved (13). Most significant is the agreement obtained by Monch and Gent (14), who measured the contact potential difference changes of a GaAs surface as a function of temperature, thereby locating the defect levels in energy and determining their density.

In their work, Brillson and co-workers used contact potential difference (Kelvin probe) and surface photovoltage (SPV) measurements to study metal-semiconductor interfaces. They conclude that Fermi level stabilization occurs over several monolayers of metal deposition, in conflict with our photoemission measurements which indicate complete stabilization for 0.1 monolayer. In their analysis, an interface "atomic dipole" layer was introduced to obtain agreement between their measurements, and larger, accepted Schottky barrier heights. This dipole, however, would be transparent to electron tunneling. Proper interpretation of their data, using the techniques of Monch et al. (15), shows that Fermi level stabilization is indeed complete by 0.1 monolayer.

In their SPV measurements, they assumed that high intensity light was sufficient to flatten the semiconductor bands. If this was correct, their SPV would measure the band bending. However, analysis using the diode equation shows that 0.43 eV of band bending remained in their case (16). Thus, their measurements are not in disagreement with the accepted barrier heights, and an atomic dipole need not be introduced.

REFERENCE PUBLICATIONS

2. W. A. Goddard, private communication.
14. W. Monch and H. Gant, to be published.

PUBLICATIONS (RECENT)

6.) Models of Column 3 and 5 Elements on GaAs (110); Application to MBE, P. Skeath, I. Lindau, C. Y. Su, and W. E. Spicer, JYST, accepted for publication as part of the PCSI-8 Proceedings, 1981.
8.) Experimental Determination of the Bonding of Column 3 and 5 Elements on GaAs, P. Skeath, C. Y. Su, I. Lindau, and W. E. Spicer. The proceedings will be published as a special issue of the Journal of Crystal Growth, Fifth International Conference on Vapor Growth and Epitaxy, Fifth American Conference on Crystal Growth, pending approval by a committee at the conference.