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19. ABSTRACT (Continue on reverse if necessary and identify by block number) Several issues of major importance for the crystal quality of mercury cadmium telluride and related materials (cadmium telluride and cadmium zinc telluride) have been investigated during the course of this contract. These issues are: the effects of defect interactions, including complex formation and possible changes in defect diffusion, the role of interstitial defects, and the magnitude and effects of lattice relaxation around defects. A new technique (the "local" matrix" method) was developed to obtain estimates of point defect total energies, electronic levels, and the character of the localized states for ionic and metallic tetrahedrally bonded materials, such as mercury cadmium telluride. Preliminary work on a more accurate tight-binding supercell method has given encouraging results.			
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INTERSTITIAL FORMATION, NON-EQUILIBRIUM AND MACROSCOPIC PROCESSES
IN MERCURY CADMIUM TELLURIDE

FINAL REPORT

C. G. Morgan-Pond

August 28, 1989

U. S. ARMY RESEARCH OFFICE

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A. STATEMENT OF THE PROBLEM STUDIED

A three year program of work, involving theoretical and computer calculations, was carried out to investigate three major issues affecting the crystal quality and long term stability of the infrared detector material HgCdTe and related alloys. The fundamental questions addressed were:

1) How do defect interactions, including the strong attraction leading to the formation of complexes, affect observed densities of simple defects and defect migration?

2) What part do interstitial-type defects play in determining electrical behavior and in non-equilibrium kinetic processes, such as diffusion?

3) How large are the force constants which determine the microscopic lattice distortion under different conditions, and how does lattice distortion affect diffusion and other defect-related properties?

Techniques used to address these questions included the calculation of equilibrium concentrations of point defects and complexes, using methods previously adapted for HgCdTe,¹ and a tight-binding small-basis, or "local matrix", treatment for estimating point defect total energies, electronic levels, and the character of the localized states, developed for covalently bonded materials with considerable ionic and metallic character, such as HgCdTe.²⁻⁵ A more quantitatively accurate tight-binding supercell approach, which can be used to investigate lattice distortion, is still under development, but has given encouraging initial results.⁶⁻⁷

During the contract period, the principal investigator was also awarded a second ARO contract (DAAL03-87-K-0061), funded in part by the

Night Vision and Electro-Optics Center (NVEOC), to use the methods developed under this contract to investigate particular problems of practical interest to NVEOC, such as the electrical inactivity of a large fraction of the In added to CdTe by non-laser-assisted molecular beam epitaxy (MBE), which is often observed.⁸ Some of the results obtained for these problems are mentioned here; a more extensive description of these results is given in the reports for Contract No. DAAL03-87-K-0061.

B. SUMMARY OF THE MOST IMPORTANT RESULTS

1. Effects of Doping and Alloying on Crystal Quality in $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$

Native point defects (vacancies, interstitials), extended defects (dislocations, precipitates, grain boundaries), and defects involving impurities are numerous in CdTe and Hg-rich HgCdTe, and tend to control the electronic properties of these materials. Previous calculations of the equilibrium concentrations of non-interacting native point defects¹ demonstrated that both CdTe and Hg-rich HgCdTe have high equilibrium concentrations of point defects during growth and annealing. In order to examine the effects of doping or substitution of small amounts of other elements, such as zinc, on crystal quality, two examples were studied: doping with indium, as a typical shallow donor, and substitution of zinc, as an isoelectronic replacement for Cd.

a. Indium Doping

Equilibrium concentrations of point defects in CdTe doped with 1.6×10^{18} and 2.7×10^{17} In/cm³ were calculated for a range of Cd overpressures and annealing temperatures.⁹⁻¹⁰ Comparison with the charge

carrier concentrations obtained in Hall experiments¹¹ showed reasonable agreement. The overall effect of adding an electrically active donor to the HgCdTe system, seen in these calculations for indium, was to reduce the equilibrium concentrations of native donor defects and to increase the concentrations of native acceptor defects. The total concentrations of native point defects were not strongly affected by addition of indium.

Calculated estimates of the binding energies of complexes formed by a charged cation vacancy or tellurium interstitial with one or two charged In donors ranged from 0.17 to 1.7 eV for $\text{Hg}_{.8}\text{Cd}_{.2}\text{Te}$ and CdTe. Although the binding energies were higher for complexes of indium with tellurium interstitials, complexes with cation vacancies were found to be dominant, due to the much greater concentrations of cation vacancies. At temperatures close to 1000K, where equilibrium may be achieved, and the comparisons with the Hall experiments on CdTe were made, complexes of one singly charged substitutional In with one doubly charged cation vacancy were the most numerous. At lower temperatures, the largest fraction of the indium condensed to form neutral complexes consisting of two substitutional In and one cation vacancy.¹² This was in agreement with results observed for $\text{Hg}_{.8}\text{Cd}_{.2}\text{Te}$, measured at 77K after annealing at 773K and 873K,¹³ where the indium was observed to be incorporated predominantly as In_2Te_3 (i. e. a complex of two In and a cation vacancy) dissolved in the HgCdTe.

These results suggested that excess tellurium, frequently present after growth in both Hg-rich material and pure CdTe, would tend to complex with the indium rather than condensing exclusively into extended defects such as dislocations or Te inclusions. However, the changes in relative equilibrium concentrations of various point defects and complexes occur gradually, and any effects on extended defect formation

should be modest. More dramatic changes in macroscopic crystal quality may arise from kinetic effects which do not require the added constituent to be charged. These effects were investigated with specific application to the isoelectronic substitution of zinc on the cation sublattice.

b. Isoelectronic Substitution: Addition of Zinc

Previous work showed that equilibrium concentrations of native point defects are not reduced substantially by adding small amounts of other elements as isoelectronic substituents, either to CdTe, or to Hg-rich HgCdTe.¹ It was argued^{1,10} that the dramatic decrease in dislocation densities seen in $\text{Cd}_{0.96}\text{Zn}_{0.04}\text{Te}$, as compared with CdTe,¹⁴ may result from strains associated with the different Cd-Te and Zn-Te bond lengths. These strains may pin the point defects generated at growth, producing a more uniform distribution of point defects and complexes, and inhibiting condensation of the point defects into larger extended defects, such as dislocations.

Since substitution of other isoelectronic elements, such as Zn, for some of the Cd appears to yield promising new materials for alternate substrates,¹⁴ it was of interest to determine whether a dramatic enhancement of interdiffusion across junctions, such as is observed on adding small amounts of Zn to the AlGaAs system,¹⁵ could occur in the HgCdTe system. The mechanism identified by Van Vechten¹⁶ for the enhancement of cation diffusion in AlGaAs, after indiffusion of Zn, involves the lowering of the activation energy for diffusion by nearest neighbor vacancy hopping, which requires the creation of antisite defects in the intermediate steps. The activation energy is reduced by the presence of highly mobile, charged Zn interstitials which can lower the Coulomb energy of the intermediate configurations. Barriers to diffusion

by various vacancy mechanisms were calculated, and it was shown that nearest neighbor vacancy hopping in CdTe and HgCdTe is always dominated by second neighbor vacancy hopping, which is relatively unaffected by the addition of small amounts of other elements.¹⁰ Therefore, it was predicted that there will be no dramatic enhancement of diffusion resulting from addition of small amounts of Zn or other elements in order to improve crystal quality.

2. Localized Defect States: Deep Levels and Total Energies

a. Development and Testing of the Local Matrix Approach

A new approach was developed for the localized states due to neutral interstitial and substitutional defects in tetrahedrally bonded semiconductors. This approach is an extension of the method,¹⁷ recently applied to self-interstitials in silicon,¹⁸ to account for the metallic coupling (s-p promotion energy) and the polar coupling, both of which are important in HgCdTe. It allows us to form a qualitative picture of the localized interstitial levels, and to investigate energy trends for the deep levels. It also gives a clear physical picture of the process of formation of the localized levels.^{5,19}

The simple model used in these calculations is based on the idea of describing the localized states within a minimal basis.²⁰ This small basis, consisting of the sp^3 bonding hybrids on the defect atom, its neighbors (which are improperly coordinated due to the presence of the defect), and all hybrids involved in covalent bonds with nearest neighbor hybrids, is separated from the rest of the crystal by the method of "soft separation",²⁻⁵ or ignoring systematically all of the weaker interactions which couple the minimal basis to the rest of the crystal. Tight-binding

interactions are included between hybrids in the minimal basis. Energy levels and wave functions for the localized states were obtained analytically for substitutional and high-symmetry (tetrahedral) interstitials. Energy levels and wave functions were obtained numerically for hexagonal interstitials.

The results of these calculations were compared with self-consistent Green's function and experimental results for various interstitials in Si and GaP,¹⁹ and for substitutional defects, including vacancies, in Si, GaP, GaAs, and CdTe.³ Agreement to within 1 eV for most levels in the vicinity of the gap, good agreement for energy trends and the general structure of the hyperdeep levels, and correct deep level symmetries and occupancies were obtained.

b. Interstitial Deep Levels

The deep levels of indium and self-interstitials (Hg, Cd, Te) in tetrahedral and hexagonal positions in $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ were characterized and energy trends were calculated within the local matrix approach.² Shifts of up to 0.5 eV were observed in the energies of specific deep levels, as the crystal composition was varied from HgTe to CdTe, due to the substitution of Cd for Hg on the cation sites in the vicinity of the interstitial. These shifts were largest for localized levels with a sizable amount of electronic charge on cations.

Several deep levels in the gap region were identified for HgCdTe. In particular, a localized level of A_1 symmetry due to a mercury interstitial in the tetrahedral position with anion nearest neighbors was identified as a possible candidate for providing midgap tunneling levels for Hg-rich HgCdTe. This is in agreement with the suggestion of Vydyanath,²¹ based on his experiments in different overpressures of

mercury, that the midgap tunneling levels in this material may be due to mercury interstitials. This particular A_1 level has a very strong cation character, with about 80% of its charge density on the interstitial and the cations bonded to its nearest neighbors.

Of the deep levels in the gap region which are due to indium interstitials, only the level of T_2 symmetry due to the indium interstitial at the tetrahedral position between cations is partially empty. In principle, this level could serve as an acceptor level, and could contribute to the overall electrical inactivity often observed for a large fraction of the indium added to CdTe by non-photoassisted MBE.⁸ Indium acts primarily as a substitutional dopant with shallow donor levels, when added in small concentrations at high temperature. However, it is known that substitutional impurities may be preferentially displaced to interstitial sites in material with high (nonequilibrium) densities of native defects resulting from radiation damage,²² and this may also occur when the high densities of native defects result from low-temperature growth.

But as will be discussed in the following section, it was found that the preferred tetrahedral position for indium interstitials is the position between anions. Therefore, tetrahedral interstitials with cation nearest neighbors should not be numerous enough to account for any substantial self-compensation. The lowest partially occupied level due to indium in the preferred tetrahedral position (and in the hexagonal position) is about 1 eV higher than the lowest partially occupied localized level obtained from the analogous calculation for substitutional indium. Even taking into account these higher energy levels, these indium interstitials are less likely to be acceptors than substitutional indium, which is known to be a shallow donor.

c. Estimates of Total Energies and Diffusion Barriers

The local matrix method was extended to obtain estimates of the total energy for interstitials at different sites in the lattice.⁴ In order to correctly represent structural energies, the short-range repulsion arising from overlap of the electron wave functions centered on neighboring atoms was included. The calculated total energy for neutral indium interstitials was higher in the tetrahedral position between cations (T1) than in the tetrahedral position between anions (T2) by about 3 eV. The T2 interstitial had an even lower energy when it was allowed to ionize to In^+ . Therefore, although T1 In interstitials have a partially filled deep level in the gap and could potentially serve as acceptors,² these interstitials should not be numerous enough to account for the electrical compensation which is seen in non-photoassisted MBE-grown films of CdTe.⁸

Results for self-interstitials showed that the T2 position was preferred for tetrahedral Hg and Cd interstitials, and the T1 position was preferred for tetrahedral Te interstitials. Therefore, tetrahedral Hg interstitials will tend to sit in T2 sites, and contribute A_1 electronic levels in the vicinity of the gap.

Experimental studies suggest that interstitials play an important role in cation diffusion in $\text{Hg}_{.8}\text{Cd}_{.2}\text{Te}^{23}$ and interdiffusion in HgTe/CdTe superlattices²⁴. The calculated total energy difference for neutral Cd interstitials in T1 and T2 positions was 8 eV, much higher than experimental activation energies. Simple interstitial diffusion through the low-electron-density channel which passes alternately through T1 and T2 sites therefore seems unlikely for Cd. It appears that diffusion of Cd interstitials must proceed by some more complicated mechanism, probably involving exchange with atoms on lattice sites. Total energy

results indicate that the open channel between T1 and T2 sites is also unlikely for In diffusion, although it may be an important channel for diffusion of Hg.

Results of this model indicate that the preferred charge state for an interstitial may change radically at different sites.^{2,4} This suggests that alternating capture and release of charge carriers by interstitials may be important in lowering energy barriers for interstitial diffusion. If interstitials are allowed to change to their preferred charge state at each site, the diffusion barriers become dependent on the Fermi level. However, the conclusions stated above are not changed: the open channel between tetrahedral sites appears to be a favorable diffusion path for Hg, less favorable for In, and quite unfavorable for Cd.

3. Supercell Calculations: Defects with Lattice Distortion

Preliminary work using a self-consistent supercell method was done for interstitials in CdTe and HgCdTe, including the effects of lattice distortion.⁶⁻⁷ We used the tight-binding model of Majewski and Vogl, which predicts semiquantitatively the lattice constants, bulk moduli, and stable structures of perfect semiconductor crystals.²⁵ Similar methods have been used by Chadi to study relaxation at surfaces,²⁶ and by Tomanek and Schluter to study the preferred structures of small silicon clusters.²⁷

For tetrahedral interstitials a simple breathing mode relaxation of the nearest neighbors outward was considered, and the total energy was minimized to find the preferred amount of lattice distortion around the defect. For hexagonal interstitials, both relaxation outward and a

possible increased puckering of the ring of neighbors surrounding the interstitial were included. Results for the relaxation about tetrahedral and hexagonal self-interstitials in silicon were generally in good agreement with results obtained using a pseudopotential density-functional method²⁸ and a self-consistent Green's function technique.²⁹ Ultimately, this method may permit calculations of total energies for complex defects including substantial lattice relaxation, with sufficient accuracy and considerably less computational effort than is necessary for self-consistent Green's function or a priori pseudopotential methods.

When the nearest neighbors were allowed to relax away from the interstitial, the on-site energies on the interstitial, and often on the neighbors as well, were reduced as the overlap between electron wave functions on the interstitial and its neighbors decreased. As a result, charge was transferred into the region containing the interstitial and the atoms nearby. In addition, the average distance between the nearest neighbors and the atoms further out to which they were bonded decreased. This contributed to the overall change in the nearest-neighbor on-site energy due to overlap. It also increased the covalent coupling and the charge transfer from cations to anions in the bonds involving the nearest neighbors. Therefore, in all cases studied, charge was transferred to the interstitial and the anions in the interstitial region, defined to include the interstitial and the neighboring atoms which were close enough to interact with the interstitial (i. e. the nearest neighbor shell for the hexagonal interstitial, and the first and second neighbor shells for the tetrahedral interstitial). There was a strong correlation between the total amount of charge transferred into this region and the optimal relaxation of the nearest neighbors outward.

For Cd, Hg, and In interstitials at the tetrahedral position between anions, the nearest neighbors moved outward by about 3% of the unrelaxed nearest neighbor distance. The main effect of this relaxation on the A_1 localized level in the gap region for the Hg interstitial was to allow this level to become more localized on the interstitial itself, and to move somewhat lower in the gap.

A considerably larger relaxation was found for the cation interstitial in the tetrahedral position between cations. This resulted from the fact that the overlap repulsion due to cation nearest neighbors was greater than the repulsion due to anion nearest neighbors. For example, the overlap contribution to the interstitial on-site energy was higher for the Cd interstitial between Cd than for the Cd interstitial between Te in CdTe. In addition, for the Cd interstitial between Cd, when the nearest neighbors relaxed away from the Cd interstitial, which made a large contribution to the nearest neighbor on-site energy, they moved toward anions further out, which made a smaller contribution. In the case of the Cd interstitial between Te, the nearest neighbors approached Cd atoms further out as they relaxed away from the Cd interstitial, and their on-site energies were increased slightly by the relaxation. The more favorable changes in both interstitial and nearest neighbor on-site energies for the cation interstitial between cations lowered the energy of the relaxed configuration, allowing the nearest neighbors of the neutral Cd interstitial between Cd in CdTe to relax outward by 6%.

There was also a substantial relaxation for the neutral hexagonal Cd interstitial in CdTe, due to the strong overlaps resulting from the larger number of nearest neighbors, at a slightly closer distance than for the tetrahedral interstitial. The six nearest neighbors relaxed

outward by about 6%, while the puckered hexagon formed by the ring of nearest neighbors increased its pucker by about 5%, measured as the fractional increase in the separation of the plane containing the three anions and the plane containing the three cations.

C. LIST OF ALL PUBLICATIONS AND TECHNICAL REPORTS

"Effects of Doping and Alloying on Defects and Complex Formation in $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ ", C. G. Morgan-Pond and R. Raghavan, Materials Science Forum 10-12, 79 (1986).

"Effects of Indium Doping and Addition of Zinc on Crystal Quality in $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ ", C. G. Morgan-Pond, Proceedings of the ARO Infrared Materials Review, Raleigh, NC, February 11-12, 1986.

"Deep Interstitial Levels in $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ ", S. Goettig and C. G. Morgan-Pond, Extended Abstracts of the 1987 MCT Workshop, New Orleans, LA, October 6-8, 1987, O/DI-27.

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"Localized States in Tetrahedrally Bonded Semiconductors", S. Goettig and C. G. Morgan-Pond, Materials Science Forum 38-41, 317 (1989)

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"Localized Interstitial States in Tetrahedrally Bonded Semiconductors - The Local Matrix Approach", S. Goettig and C. G. Morgan-Pond, in preparation.

D. LIST OF ALL PARTICIPATING SCIENTIFIC PERSONNEL
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