HgTe-CdTe SUPERLATTICES

D.L. Smith and T.C. McGill

California Institute of Technology, Pasadena, California 91125, U.S.A.

Résumé— Nous présentons une étude théorique se rapportant aux propriétés électroniques des super-réseaux HgTe-CdTe. Nous calculons, en fonction de la période du super-réseau, les valeurs de gap d'énergie, de masses effectives normales aux interfaces et de longueurs caractéristiques d'effet tunnel. Les mêmes quantités sont aussi calculées pour un alliage (Hg,Cd)Te et comparées avec celles obtenues pour le super-réseau HgTe-CdTe. Il est démontré qu'en général, les super-réseaux HgTe-CdTe possèdent des propriétés supérieures à celles des alliages pour les applications en détection infra-rouge.

Abstract— We report on a theoretical study of the electronic properties of HgTe-CdTe superlattices. The band gap as a function of layer thickness, effective masses normal to the layer plane and tunneling length are compared to the corresponding (Hg, Cd)Te alloys. We find that the superlattice possesses a number of properties that may make it superior to the corresponding alloy as an infrared material.

1-Introduction

Superlattices formed of HgTe and CdTe have been proposed as materials for application in the infrared /1-3/. In the last couple of years a number of groups have made serious attempts to fabricate these superlattices /4-6/.

In elemental and alloy based ($\text{Hg}_x\text{Cd}_{1-x}\text{Te}$ — $\text{Hg}_y\text{Cd}_{1-y}\text{Te}$) superlattices, the material is made up of alternating layers of the compounds or alloys. The simplest case is illustrated by concentrating on the elemental superlattice. In this case, the superlattice can be viewed in a Kronig-Penney square well model like that schematically illustrated in Fig. 1. In drawing this figure, the valence band offset has been taken to be zero. This value is consistent with all of the measured results and the few empirical ideas for estimating valence band offsets /7,8/. In this schematic the holes do not experience a barrier in going from one layer to another. However, the electrons see the full difference in the band gaps. As noted originally in Ref. 1, this superlattice has the property that the band gap is dependent on thickness of the layers. In the limit of very thick HgTe layers the band gap is zero since it originates in the HgTe. As the thickness of the HgTe layer is reduced, the band gap increases as a result of the confinement of the conduction band wavefunction. In the limit of very thin layers the superlattice bandgap approaches that of the alloy with the same composition. Another property of such a structure was noted in the original papers by Schulman and McGill /1-3/. The close proximity of the valence band edge of CdTe implies that the tunneling length in the CdTe for electrons at the conduction band edge is quite long and that the masses for electrons at the conduction band edge normal to the layers is relatively small. For thinner CdTe layers, the superlattice can behave as a three-dimensional bulk materials as opposed to the two dimensional character of many of the other materials and systems.

In this paper we report on a more accurate study of the near band edge properties of the HgTe-CdTe superlattices and make detailed comparisons with the corresponding properties of

Fig. 1- Schematic illustration of the HgTe-CdTe heterojunction. Repetition of this heterojunction produces the superlattice. The valence band offset is taken to be zero.

the alloys. Section II contains a brief description of the theoretical technique used to make the calculations. Section III gives the results and compares them with those corresponding to the alloys. Section IV presents our conclusions.

II-Calculational Method

In the original papers by Schulman and McGill /1-3/, the calculations were carried out using the empirical tight-binding technique. This technique had one deficiency in that it aimed at reproducing the optical transitions for the HgTe and CdTe but did not give an accurate description of the near band edge properties such as effective masses. In this report, we give the results of k-p calculations that reproduce the near band edge properties very accurately. The calculational approach is similar to those reported by White and Sham /9/, and Bastard /10/. A two-band k-p approach is applied to the conduction and light hole band. The heavy hole band is also treated using this formalism. It is taken to connect through the momentum matrix element with the Γ_{15} conduction band states. The potential is assumed to be constant in the two layers with a discontinuity at the interface for the s-like potential (the conduction band offset). An analytical expression for the superlattice energy-wavevector relation is obtained. The alloy is also described using a 2-band k-p approach. The parameters in the k-p are obtained using a virtual crystal type approximation.

The splittings $\Gamma_8-\Gamma_8$ and $\Gamma_{15;c}-\Gamma_8$ are taken to be 1.60 eV and 6.01 eV for CdTe and -0.303 eV and 5.58 eV for HgTe. The Γ_6 to light hole momentum matrix element is taken to be $2.54\sqrt{eV m_0}$ and the $\Gamma_{15;c}$ to heavy hole matrix element is taken to be $2.30\sqrt{eV m_0}$, resulting in a heavy hole effective mass of $0.55m_0$ in both materials. The lattice constant was taken to be 6.472 Å. The valence band offset was taken to be zero.

The effective masses are obtained by differentiating the resulting energy-wavevector relation. The tunneling length is obtained by finding the imaginary superlattice wavevector in the bandgap of the superlattice.

III-Results

In Fig. 2 we present the results for cutoff wavelength as a function of composition for the alloy and layer thickness for superlattices in which the thickness of the HgTe is the same as the CdTe. The result for the alloy shows the characteristic singularity at $x = 0.14$. In contrast the result for the bandgap of the superlattice shows no such singularity. The cutoff wavelength smoothly approaches infinity as the thickness of the HgTe layer approaches infinity. This result implies an obvious advantage for the superlattice. To reach a given cutoff wavelength, the parameters which must be controlled are the thickness of the layers. Since in the case of the superlattice the cutoff wavelength is not singular in this parameter, the precision with which this parameter must be controlled to reach a given cutoff is much less in the superlattices than in the alloys.

Fig. 2- The cutoff wavelength or the reciprocal of the bandgap for the alloy as a function of composition and the superlattice as a function of layer thickness. The thicknesses of the HgTe and CdTe layers in the superlattice are assumed to be the same.

One characteristic of narrow-band-gap, zincblende-crystal-structure material is the very small effective mass [11]. In Fig. 3, we have plotted the effective mass of the conduction band for the alloy and the superlattice normal to the layers as function of the cutoff wavelength or the reciprocal of the band gap. To illustrate our point the results for equal HgTe and CdTe layer thicknesses are presented. This figure shows a very interesting property of the superlattice as compared to the alloy. The effective mass of the superlattice is much larger than that for the corresponding alloy.

In most device structures employing narrow band gap semiconductors, the very small electron effective mass is an obvious disadvantage. The small effective mass leads to large diffusion currents and large tunneling currents through the depletion region of the devices. In the case of the superlattices the effective mass and the band gap are not strongly coupled. Hence, one can obtain values for the effective mass in the appropriate direction that are large compared to those for the same band gap in the alloy.

To illustrate this point quantitatively, we have plotted a characteristic length governing the tunneling as a function of the cut-off wavelength for a superlattice and alloy in Fig. 4. We have selected the characteristic length to be the reciprocal of the imaginary part of the wavevector at its maximum in the forbidden gap. Again for convenience we have chosen the case when the superlattice is made of layers of HgTe and CdTe with the same thickness. The important point to note from this figure is the rather large values of the tunneling length for the alloy that are obtained when the cut-off wavelength is large and the rather small values that are obtained in the superlattice.

IV-Conclusions

In this short note we have presented an accurate study of the narrow band edge properties of the HgTe-CdTe superlattices. The theoretical results suggest three very important properties of this superlattice as an infrared material: First, the band gap is continuously adjustable from the value of the alloy to zero for a fixed ratio of HgTe to CdTe. Second, for moderate

Fig. 3- The electron effective mass as a function of the cutoff wavelength for the alloys and a superlattice with equal thicknesses of HgTe and CdTe. The effective mass for the superlattice is that normal to the layers. Note the scale change on the effective masses for the two graphs.

Fig. 4- The tunneling length as a function of cutoff wavelength for the alloy and superlattice. The tunneling length is defined to be the reciprocal of the imaginary part of the wavevector at its maximum if the forbidden gap. The superlattice consists of HgTe layers and CdTe layers with the same thickness.

thicknesses of the CdTe layers, the superlattice can behave as a three-dimensional material with a reasonable value for the mass of the electrons normal to the layer. Third, the electron tunneling is significantly reduced compared to that for the alloy of the same bandgap.

These properties make the superlattices of HgTe-CdTe one of the most exciting recent developments in infrared materials.

Acknowledgement

The authors gratefully acknowledge the support of the United States Army Research Office under Contract No. DAAG-80-C-0103.

References

1. Schulman, J. N. and McGill, T. C., *Appl. Phys. Lett.* **34** (1979) 663 .
2. Schulman, J. N. and McGill, T. C., *J. Vac. Sci. Technol.* **16** (1979) 1513.
3. Schulman, J. N. and McGill, T. C., *Phys. Rev.* **B23** (1981) 4149.
4. Faurie, J. P., Million, A., and Piagnet, J., *Appl. Phys. Lett.* **41** (1982) 713.
5. Chow, P. P., Greenlaw, D. K., and Johnson, D., *J. Vac. Sci. Technol.* **A1** (1982) 562.
6. Cheung, J. T. **Proceedings of the HgCdTe Workshop** *J. Vac. Sci. Technol.* (to be published).
7. Kuesch, T. F. and McCaldin, J. O., *J. Appl. Phys.* **53** (1982) 3121.
8. Faurie, J. P., **Proceedings of Electronic Materials Conference 1983** *J. Electronic Materials* **13** (to be published).
9. White, S. R. and Sham, L. J., *Phys. Rev. Lett.* **47** (1981) 879.
10. Bastard, G., *Phys. Rev.* **B25** (1982) 7584.
11. C. Kittel, **Quantum Theory of Solids** (John Wiley and Sons, Inc., New York, 1963) pp. 186ff.