Superlattices: Progress and prospects

T. C. McGill, G. Y. Wu, and S. R. Hetzler
T. J. Watson, Sr., Laboratory of Applied Physics, California Institute of Technology, Pasadena, California 91125

(Received 15 December 1985; accepted 13 March 1986)

The current status of HgTe–CdTe superlattices is reviewed. The properties predicted for the superlattices have been studied qualitatively in the cases where both theory and experiment exist. In particular, it has been found by both infrared absorption and photoluminescence that band gaps of the superlattices are substantially less than those of the alloy with the same average composition. Theoretical studies have concentrated on the factors (strain, band offsets, interdiffusion) that could result in substantial deviation of the properties of the superlattices from those predicted by the original simple theories. Some of the areas requiring further development are reviewed and discussed.

I. INTRODUCTION

Since the original proposal of HgTe–CdTe superlattices as a new infrared material,[1] a great deal of interest has developed in the proposal. Smith and co-workers[2] have pointed out some of the advantages that this material could have over alloys for application in infrared devices, particularly those operating at wavelengths beyond 10 μm. The band gaps (cutoff wavelength) of the superlattices are likely to be much easier to control than the alloy. Leakage currents in narrow band gap structures are likely to be reduced by orders of magnitude in the superlattice over those in the alloys.

In the superlattice, the band gap (E_G) is controlled by the thickness of the layers. By contrast in the alloy, the band gap is controlled by the composition of the material, the relative Hg to Cd ratio. The band gap of the alloy goes to zero at some finite value of this ratio. Hence, the cutoff wavelength ($\lambda_C \propto 1/E_G$) exhibits a singularity at the composition ratio where E_G goes to zero. To have adequate control of the cutoff wavelength, one has to have progressively better control of the composition ratio as one goes to longer and longer cutoff wavelengths. On the other hand, for the superlattice, the cutoff wavelength is a smooth, slowly varying function of the layer thicknesses. Hence, it is easier to obtain the desired value of the band gap.

In the zinc blende, narrow-band-gap semiconductors, the effective mass of the light hole band and the conduction band are directly proportional to the band gap.[3] Hence, as the band gap becomes small, the effective masses also become small. This, of course, improves the various transport parameters, but, at the same time, it increases the leakage current through depletion regions in devices formed from this material. The superlattice to some degree decouples this relation between effective mass and band gap. The effective mass for transport normal to the layers can be made large even when the band gap is small. Hence, the leakage current can be made quite small even when the band gap is small. A simple calculation for a cutoff wavelength of 20 μm indicates that the leakage current could be reduced by orders of magnitude. Following the first success in fabricating these structures by Faurie and co-workers,[4] Cheung[5] and Chow[6] also reported success in fabricating HgTe–CdTe superlattice. All of these successes were obtained by using either molecular-beam epitaxy or a laser stimulated version of MBE. Most of the early studies consisted of structural characterization of the superlattices with relatively thick layers. However, as of the time of the last workshop[7,8] the all important near band gap properties of these systems were beginning to be explored. Attempts to determine the band gap from infrared absorption measurements suggested that the measured values of the gap were in substantial disagreement with the theory. In fact, the band gaps were coming out nearer the alloy than the values predicted by various theories.

The work over the last year has been aimed heavily at clarifying this situation. The theorists have examined various aspects of the predictions to give some bounds on the band gaps that could be obtained. The experiments have been aimed largely at obtaining better values for the band gaps in the superlattices and to make more detailed comparisons between theory and experiment.

In this manuscript, we will review some of the important developments in theory and experiment and indicate where we think future work will be important.

II. THEORY

The first question is: Do HgTe–CdTe superlattices behave in the way one would expect for a typical semiconductor for application in the infrared? Does it have a direct band gap, and how big is the optical absorption? In Fig. 1, we present the results of a calculation of the band structure of a superlattice. The dispersion both parallel and perpendicular to the layers is presented. The calculations were carried out using a so-called 8 band $k\cdot p$ calculation. The 8 bands were the 4 Γ_8 bands, the 2 Γ_6 bands, and the 2 Γ_7 bands.[9] The calculation was carried out for 14 layers of HgTe and 4 layers of CdTe. The band offset is taken to be 40 meV[10] and the strain in the layers is taken to be zero. In this figure, the states with energy less than zero are occupied (the valence bands), and states with energy greater than zero are empty (the conduction bands). The band structure has all of the characteristics that one might expect for a typical material. It has a band gap at the position shown. The valence bands turn down, producing a semiconductor. Decomposition of the wave function into component parts indicates that the Γ_6 as well as the Γ_8 components of the wave function are very important. Calcu-

 0734-2101/86/042091-05$01.00

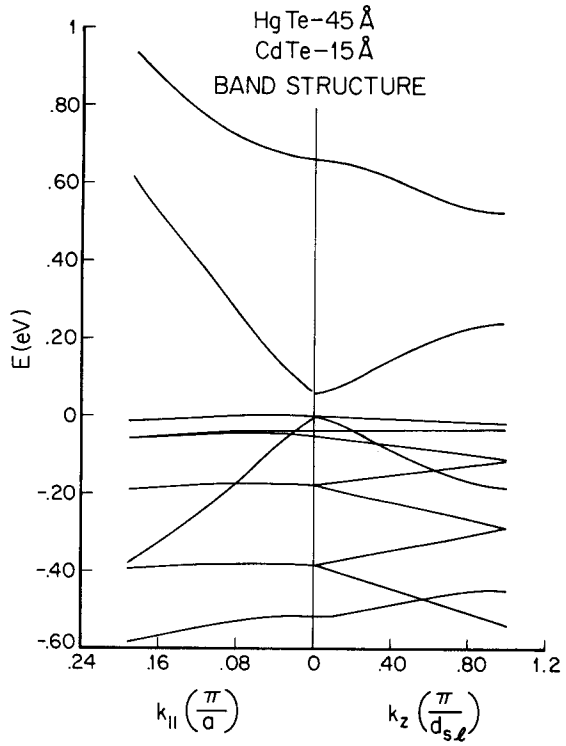

FIG. 1. Band structure of a representative superlattice. The zero of energy is taken to be the valence band edge. Dispersion for wave vectors perpendicular to the layers k_z (measured in units of π/d_{sl}, where d_{sl} is the total thickness of each repeat of the superlattice, 60 Å in this case) and for wave vectors parallel to the layers $k_{\parallel}$ (measured in units of π/a, where a is the lattice constant of bulk HgTe, approximately 6.46 Å). The method used in calculating the band structure is given in the text.

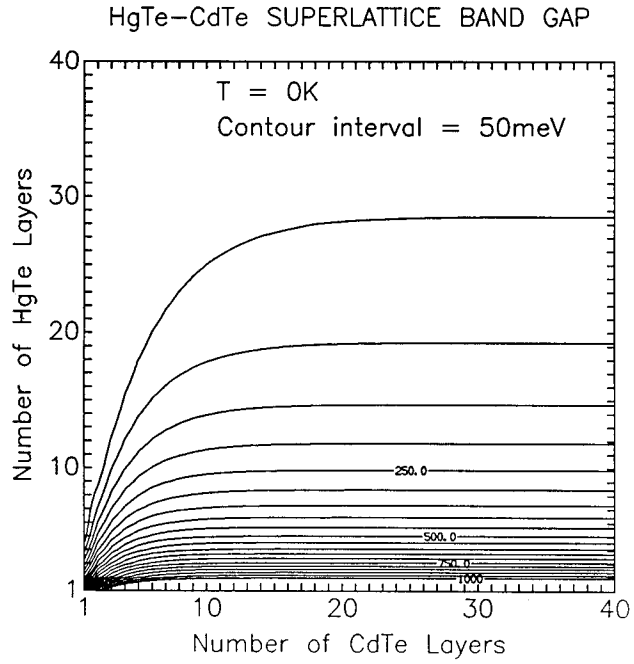

FIG. 2. Contour plot of the band gap of HgTe–CdTe superlattices at a temperature of 0 K. The calculations were carried out using a technique described in the text.

lations like those reported by Lin-Liu and Sham[11] that do not include Γ_6 are not capable of producing the correct behavior of the wave function and, hence, produce erroneous electronic spectra. The importance of the Γ_6 component of the wave function near the band edge in the superlattice has been confirmed by calculations by Cade.[12]

In Figs. 2, 3, and 4, we have presented contour plots of the band gap of superlattices as a function of the thickness of the HgTe and CdTe layers. The calculations presented in these figures assume that there is no strain in the HgTe or CdTe layers. The band offset is assumed to be 40 meV.[10] The calculations are carried out using the Bastard model,[13] using the parameters given in Ref. 2. The temperature dependence was calculated using temperature dependence of the bulk band gaps[14] obtained from Ref. 15. The band gap as a function of thickness is shown in Fig. 2 for 0 K, in Fig. 3 for 100 K, and in Fig. 4 for 300 K. The results in these figures can be used as a guide to picking the thickness of layers for obtaining a given band gap. The results show that a band gap of the superlattices is largely determined by the thickness of the HgTe layers and not the thickness of the CdTe layers when the thickness of the CdTe layers is sufficiently large.

The large Γ_6 and Γ_8 components in the wave function result in significant optical absorption, since the appropriate matrix element between these components is quite large.[16] The values of $\epsilon_2(\omega)$ are comparable to those obtained for the alloys.

Most of the recent theoretical work has been aimed at exploring the variation of properties due to changes in the parameters in the theory. Schulman and Chang[17] have examined the role of interdiffusion on the band gaps of the superlattice. Perfectly abrupt superlattices have band gaps that are less than the alloy that has the same average composition. Hence, overall as we go from the perfectly abrupt superlattice to the completely interdiffused superlattice, the alloy, the band gap increases. This trend of increasing gaps

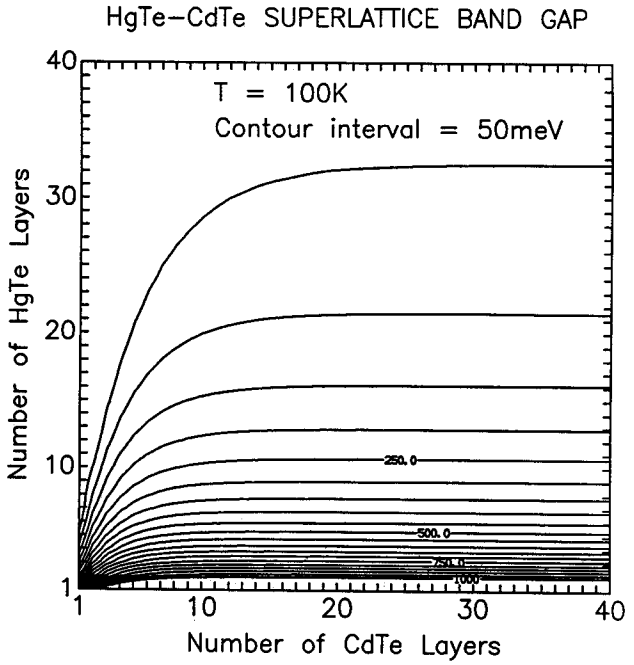

FIG. 3. Contour plot of the band gap of HgTe–CdTe superlattices at a temperature of 100 K. The calculations were carried out using a technique described in the text.

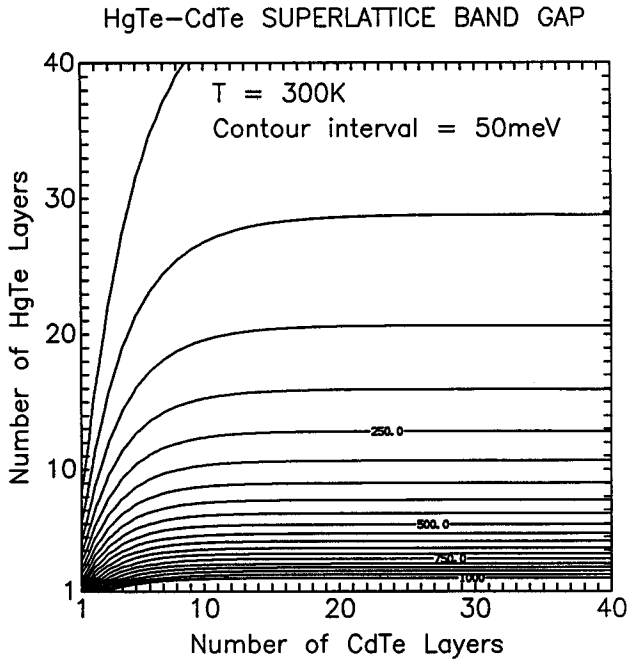

FIG. 4. Contour plot of the band gap of HgTe–CdTe superlattices at a temperature of 300 K. The calculations were carried out using a technique described in the text.

has been shown by some simple model calculations in Ref. 17.

The character of the states at the band edge of the superlattice is very important. Recently, the character of the states at the band edge has been examined in detail by Chang *et al.*[18] They have found that the states in the HgTe–CdTe superlattice are a bit different from those in other superlattices and heterojunctions. The Γ_8 components of the wave function are strongly localized at the interface. However, the Γ_6 portion of the wave function behaves in the standard way with a peak at the center of the HgTe quantum well produced by the CdTe barriers on either side. The relative contribution of Γ_6 and Γ_8 to the wave function depends on the thickness of the layers in the superlattice. In the limit of very thick HgTe layers, the Γ_6 contribution becomes very small, and the interface contribution dominates. However, for superlattices in the 8–14 and the 18–22 μm regions, the Γ_6 contribution is rather large, and the results are not heavily interfacelike.

One of the principal parameters for heterojunctions is the band offset. This parameter describes the relative lineup of the band edges at the interface. In the case of the HgTe–CdTe heterojunction, the band offset is still somewhat uncertain. Based on the common anion rule,[19] the offset in the valence band should be very small, and the full band gap difference should appear in the conduction band edge:

$$\Delta E_V = E_V^{\mathrm{HgTe}} - E_V^{\mathrm{CdTe}} \approx 0 ,$$

$$\Delta E_C = E_C^{\mathrm{CdTe}} - E_C^{\mathrm{HgTe}} \approx E_g^{\mathrm{CdTe}} - E_g^{\mathrm{HgTe}} .$$

However, recently significant deviations from the common anion rule have been reported for GaAs–AlAs.[20] On the experimental side, Kuech and McCaldin,[21] working with heterojunctions grown by metal–organic chemical-vapor deposition, set a bound on the valence band offset of $\Delta E_V < 0.6$ eV. Measurements of the band offset by Johnson, McCaldin, and McGill[22] on heterojunctions grown by a low-temperature, liquid-phase-epitaxy process set a slightly lower bound of $\Delta E_V < 0.5$ eV. Interpretation of magneto-optical absorption data on HgTe–CdTe superlattices[10] has given an estimate of the band offset for the valence band of $\Delta E_V \approx 40$ meV.

In summary, the value of the band offset is not known definitely. Hence, it is important to ask how much the properties vary as a function of band offset. In Fig. 5, we have the variation of the band gap of a superlattice with band offset for a number of different CdTe thicknesses.[23] The important feature of this curve is that the band gap is a maximum at $\Delta E_V = 0$. The band gap decreases both for increasing and decreasing values of ΔE_V. The variation of the gap is slow, and the gaps would not be substantially different from the value obtained at $\Delta E_V = 0$.

The two compounds making up the HgTe–CdTe superlattice have lattice constants which differ by 0.3%. Hence, it is not possible to fabricate superlattices without some strain in the layers. Many of the superlattices are grown on CdTe substrates. Fabrication on a CdTe substrate will result in all of the strain being in the HgTe layers. Calculations by Wu and McGill[24] indicate that strain makes little change in the band gap and optical properties of superlattices with band gaps larger than few 10's of meV but does make changes in the valence band structure. Strain may be particularly important in developing an understanding of the transport properties associated with holes and the magnetoptical experiments on superlattices with thick layers of HgTe.[10]

In summary, most of the effort has been aimed at examining various aspects of the original calculations of the properties of the superlattices to see what range of properties might be observed. To date, the theorists have come up with changes in the properties that could both increase and de-

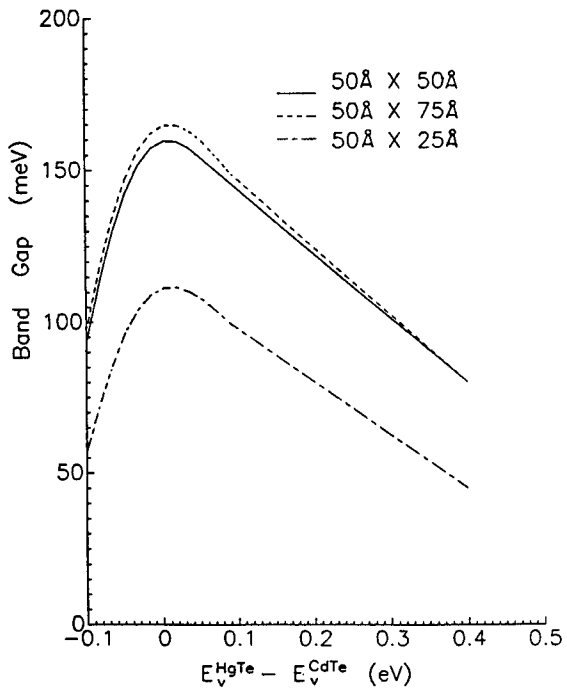

FIG. 5. Variation of the band gap of a few superlattices with the band offset in the valence band $E_V^{\mathrm{HgTe}} - E_V^{\mathrm{CdTe}}$ (after Ref. 23).

crease the band gap of the superlattice. However, without substantial interdiffusion, it is unlikely that the band gap of the superlattice will be close to that for the alloy with the same composition as the average composition of the superlattice.

III. EXPERIMENTAL STUDIES

Experimental studies of superlattices are continuing. As noted in the Introduction, most of the effort has been aimed at determining whether the near band edge optical properties are in close agreement with what has been predicted by the theory and what would be measured experimentally. The near band edge optical properties[25] and the infrared photoluminescence spectra[26] have been measured.

The infrared absorption spectra on a number of superlattices have been measured by Jones, *et al.*[25] They fit the observed absorption to

$$\alpha(\omega) = \alpha_0(\hbar\omega - E_{\text{gap}})^p .$$

The values of α_0 and E_{gap} are adjusted to obtain the base fit to the data for various values of the exponent p. The values of the gap obtained by this procedure are relatively independent of temperatures from 30 to 300 K for most of the superlattices studied. The values of the band gaps obtained from this procedure are in substantial disagreement with the theory. However, the experiment is difficult to interpret. The superlattice samples are made up of a number of layers with different dielectric properties, resulting in Fabry–Perot resonances in the transmission and reflection spectra. The thickness of the absorbing layer is quite small, on the order of 1 μm. To obtain substantial changes in the transmission, one needs values of the absorption that are on the order of 10^4 cm^{-1}. This value of the absorption is reached only for values far into the absorption edge.[16,27] These two facts make it difficult to get accurate values for the absorption from the infrared transmission and reflection experiments.

The infrared photoluminescence spectra of two superlattices have recently been published.[26] A typical infrared photoluminescence spectra for a superlattice and a comparable alloy is presented in Fig. 5. The photoluminescence shows a single asymmetric peak. The position of the peak shifts with temperature, but the shape is relatively insensitive to pump power. The position of the peak as a function of temperature is shown in Fig. 6. To show a comparison with the results obtained from the theory, we have also plotted the theoretical results obtained for various numbers of HgTe and CdTe layers (Fig. 7). The sum of the HgTe and CdTe layers was held constant at a value in agreement with the total thickness and number of repeats grown. As can be seen, the experimental positions are substantially different from those expected for the alloys. The measured positions are in reasonable agreement with the expected theoretical values.

IV. FUTURE DIRECTIONS

Projections into the future are usually wrong. However, it can be stated with some accuracy some of the important points that need to be resolved.

Interdiffusion of the HgTe and CdTe looms as one of the serious potential limitations to fabricating arbitrary HgTe–

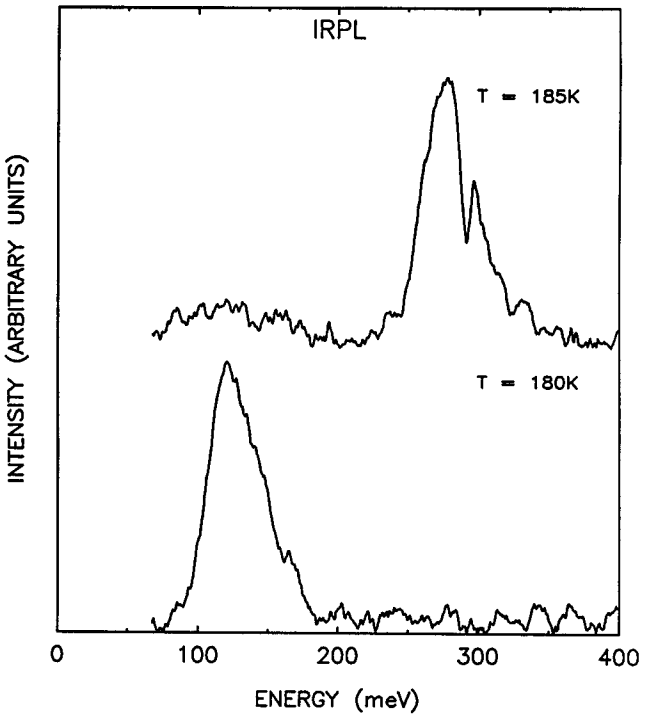

FIG. 6. Infrared photoluminescence (IRPL) spectrum for a HgTe–CdTe superlattice. The superlattice was grown by Faurie to nominally have layer thicknesses of 18–20 Å of CdTe and 40–42 Å of HgTe. The superlattice consisted of 250 repeats. For a more complete description of the superlattice see Ref. 27. For comparison we have also shown the IRPL spectrum from an alloy with approximately the same composition as the average composition of the superlattice.

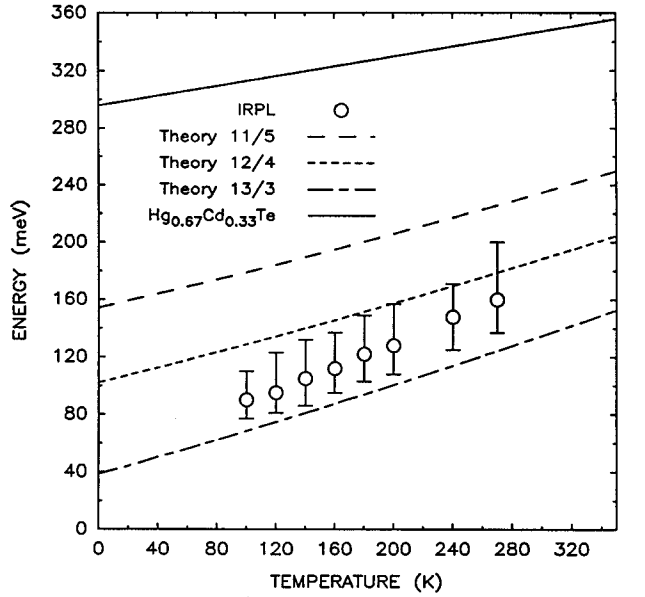

FIG. 7. Temperature dependence of the infrared photoluminescence spectra for the superlattice described in Fig. 6. The dots are the position of the peak in the spectra. The bars indicate the position of the half-maximum peaks. For comparison we have plotted (the solid line) the temperature dependence of an $Hg_x Cd_y Te$ alloy. The variation of the band gap with temperature for superlattices with the number of HgTe layers and CdTe layers given by the ratios labeling the broken lines are also plotted. The results for the superlattices were obtained from the theory used to produce Figs. 2–4 and described in the text.

CdTe superlattices. At present, our understanding of the interdiffusion of the HgTe and CdTe is not sufficient to allow us to make useful predictions as to what limitations interdiffusion will present.

Doping in superlattice structures, such as the HgTe–CdTe superlattice, is a very interesting topic. The kind of doping that we can obtain has yet to be clearly determined. The HgCdTe alloys are usually dominated by intrinsic defect doping. The big question is: What will this doping be like in the case of superlattices? What kinds of defects can we hope to obtain in these structures? The position of the defect, either in the CdTe or HgTe layer, could produce quite different results as far as doping. The questions associated with extrinsic doping have not been explored as well.

We have only begun to explore the transport properties of these superlattices.[7,28] The predicted advantage of low leakage current for superlattices over the alloy has yet to be demonstrated.

Improvements in our understanding of the HgTe–CdTe heterojunction are going to be required. Many of the transport properties of the superlattice involving motion of the carriers normal to the layers are relatively sensitive to the value of the band offset. Hence, studies of the band offset can give us new confidence in the value of the band offsets.

In general, the theory of these structures needs continuing development. At present, we are still beginning to learn how to describe the electronic spectra near the band edge. However, we have not explored any of the properties of phonons, scattering mechanisms, properties of dopants, and device physics.

Finally and most importantly, we have not made studies of how these HgTe–CdTe superlattices would be used in devices. The whole question of what a device involving a HgTe–CdTe superlattice would look like has not been addressed. We also have to address the question of what kind of processing would be required to attain such a device and what kind of processing steps are consistent with maintaining the composition modulation of a superlattice. Such natty questions as Ohmic contacts and noise have not been explored at all.

V. SUMMARY

We are at a very early stage in the exploration of HgTe–CdTe superlattices. The first experiments are extremely heartening in that the properties that are being observed lead one to believe that we are fabricating superlattices, and these superlattices have properties qualitatively like those suggested by the theories. We are still a long way from having a level of understanding of these HgTe–CdTe superlattices that rival the level of understanding for the alloys. However, based on the initial successes, it seems worthwhile to continue to explore the properties of these systems with an eye to incorporating them into various infrared applications.

ACKNOWLEDGMENTS

The work at Caltech on HgTe–CdTe superlattices has been supported from the beginning by the Army Research Office, most recently under Contract No. DAAG 29-83-K-0104. One of us (TCM) has profited from discussions with a whole host of investigators in the field including: J. N. Schulman (Hughes Research Laboratories), D. L. Smith (Los Alamos Scientific Laboratories), J. O. McCaldin (Caltech), C. Mailhiot (Xerox), A. Hunter (Hughes Research Laboratories), J. Baukus (Hughes Research Laboratories), J. P. Faurie (University of Illinois at Chicago), P. Chow (Perkin Elmer), O. Marsh (Hughes Research Laboratories), C. Jones (Santa Barbara Research Center), T. N. Casselman (Santa Barbara Research Center), M. Kinch (Texas Instruments), G. Roberts (Texas Instruments), and J. Ballingall (McDonnell Douglas).

[1]J. N. Schulman and T. C. McGill, Appl. Phys. Lett. **34**, 663 (1985).
[2]D. L. Smith, T. C. McGill, and J. N. Schulman, Appl. Phys. Lett. **43**, 180 (1983).
[3]C. Kittel, *Quantum Theory of Solids* (Wiley, New York, 1963), p. 283.
[4]J. P. Faurie, A. Million, and J. Piaguet, Appl. Phys. Lett. **41**, 713 (1982).
[5]J. T. Cheung, J. Bajaj, and M. Khoshnevisan, in Proceedings of Infrared Information Symposia, Detector Speciality Meeting, Boulder, 1983.
[6]P. P. Chow, D. K. Greenlaw, and D. Johnson, J. Vac. Sci. Technol. A **1**, 562 (1983).
[7]J. P. Faurie, M. Boukereche, J. Reno, S. Sivananthan, and C. Hsu, J. Vac. Sci. Technol. A **3**, 55 (1985).
[8]P. P. Chow and D. Johnson, J. Vac. Sci. Technol. A **3**, 67 (1985).
[9]C. Mailhiot, D. L. Smith, and T. C. McGill, J. Vac. Sci. Technol. B **2**, 371 (1984).
[10]Y. Guldner, G. Bastard, J. P. Vieren, M. Voos, J. P. Faurie, and A. Million, Phys. Rev. Lett. **51**, 907 (1983).
[11]Y. R. Lin-Liu and L. Sham, Phys. Rev. B **32**, 5561 (1985).
[12]C. Cade, J. Phys. C **18**, 5135 (1985).
[13]G. Bastard, Phys. Rev. B **25**, 7584 (1982).
[14]Y. Guldner, G. Bastard, and M. Voos, J. Appl. Phys. **57**, 1403 (1985).
[15]J. Chu, S. Xu, and D. Tang, Appl. Phys. Lett. **43**, 1064 (1983).
[16]G. Y. Wu, C. Mailhiot, and T. C. McGill, Appl. Phys. Lett. **46**, 72 (1985).
[17]J. N. Schulman and Y. C. Chang, Appl. Phys. Lett. **46**, 571 (1985).
[18]Y. C. Chang, J. N. Schulman, G. Bastard, Y. Guldner, and M. Voos, Phys. Rev. B **31**, 2557 (1985).
[19]J. O. McCaldin, T. C. McGill, and C. A. Mead, Phys. Rev. Lett. **36**, 56 (1976).
[20]Geoffrey Duggan, J. Vac. Sci. Technol. B **3**, 1224 (1985).
[21]T. F. Kuech and J. O. McCaldin, J. Appl. Phys. **53**, 3121 (1981).
[22]M. B. Johnson, A. Zur, J. O. McCaldin, and T. C. McGill, J. Vac. Sci. Technol. B **3**, 1260 (1985).
[23]G. Y. Wu and T. C. McGill, J. Appl. Phys. **58**, 3914 (1985).
[24]G. Y. Wu and T. C. McGill, Appl. Phys. Lett. **47**, 634 (1985).
[25]C. E. Jones, J. P. Faurie, S. Perkowitz, J. N. Schulman, and T. N. Casselman, Appl. Phys. Lett. **47**, 140 (1985).
[26]S. R. Hetzler, J. P. Baukus, A. T. Hunter, J. P. Faurie, P. P. Chow, and T. C. McGill, Appl. Phys. Lett. **47**, 260 (1985).
[27]J. P. Baukus, A. T. Hunter, O. J. Marsh, C. E. Jones, G. Y. Wu, S. R. Hetzler, T. C. McGill, and J. P. Faurie, J. Vac. Sci. Technol. A **4**, 2110 (1986).
[28]F. J. Boero, N. P. Ong, and J. T. Cheung, Solid State Commun. **54**, 35 (1985); N. P. Ong, G. Kote, and J. T. Cheung, Phys. Rev. B **28**, 2289 (1983).