

MARSHALL
GRANT
IN-76-CR
53309
P-39

SEMI-ANNUAL REPORT

TITLE OF GRANT

Further Improvements in Program to Calculate Electronic Properties of Narrow Band Gap Materials

TYPE OF REPORT

Brief Summary of Project

NAME OF PRINCIPAL INVESTIGATOR

James D. Patterson

James D. Patterson
Dec. 15, 1991

PERIOD COVERED BY THE REPORT

June 15, 1991 - December 15, 1991

NAME AND ADDRESS OF GRANTEE INSTITUTION

Florida Institute of Technology
150 W. University Boulevard
Melbourne, FL 32901

GRANT NUMBER

NAG8-781 Supplement 2 ✓

George C. Marshall Space Flight Center
Marshall Space Flight Center, AL 35812
(Technical Officer Sandor L. Lehoczky, ES75)

(NASA-CR-189503) FURTHER IMPROVEMENTS IN
PROGRAM TO CALCULATE ELECTRONIC PROPERTIES
OF NARROW BAND GAP MATERIALS Semiannual
Report, 15 Jun. - 15 Dec. 1991 (Florida
Inst. of Tech.) 39 p

N92-13813

Unclas
0053309
CSCL 20L G3/76

Personnel

James D. Patterson, Principal Investigator
Professor and Head, Physics and Space Sciences Department
Florida Institute of Technology

Wafaa Abdelhakiem Gobba, Post Doctoral Research Associate
Physics and Space Sciences Department
Florida Institute of Technology

Brief Summary

**“Further Improvements in Program to Calculate Electronic
Properties of Narrow Band Gap Materials”**

- I. List of Tasks Accomplished
- II. List of Reports and Papers
- III. Appendix: Abstracts of Papers and Talks

I. LIST OF TASKS ACCOMPLISHED

1. Characterization of Donors and Acceptors

The study of donors and acceptors in narrow gap semiconductors is by no means simple. Misplaced Hg in MCT seem to be the cause of intrinsic doping. Hg vacancies can produce p type materials and Hg interstitials n type. Indium doping has caused p type MCT to become n type as expected. It is possible to have both deep levels and shallow states. The deep levels can be caused by interstitials and if we neglect them we are left with the shallow levels that, at least for small x, can merge with the conduction band. We can understand this merger as related to the Mott transition. When the density of defects increases, discrete energy levels become broadened and produce energy levels that may join with the energy band. In fact it has been predicted that $\text{Hg}_{0.8}\text{Cd}_{0.2}\text{Te}$ with a donor concentration of at least 10^{14} cm^{-3} would not have bound states and this seems to be well confirmed experimentally. In general there appears to be no carrier freezeout for bandgaps in MCT which have $x < .2$. The following references seem to be relevant.

REFERENCES

1. E. Erbarut, "Electronic Structure of the Ideal Vacancies in (Hg, Cd) Te," *phys. stat. sol. (b)* 164, 235-241 (1991).
2. I.M. Tsidilkovski, G.I. Harus and N.G. Shelashina, "Impurity States and Electron Transport in Gapless Semiconductors," *Advances in Physics* 34, 43-174 (1985).
3. M.A. Berding, M. van Schilfgaarde, A.T. Paxton, and A. Sher, "Defects in ZnTe, CdTe, and HgTe: Total Energy Calculations," *J. Vac. Sci. Technol. A* 8(2) 1103-1107 (1990).
4. C.L. Littler, D.G. Seiler, and M.R. Loloee, "Magneto-optical Investigation of Impurity and Defect Levels in HgCdTe Alloys," *J. Vac. Sci. Technol. A* 8(2), 1133-1138 (1990).

5. J.B. Choi and H.D. Drew, "Donor Spectroscopy in $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ a High Magnetic Fields," Phys. Rev. B. 41, 8229-8239 (1990).
6. P. Capper, "A Review of Impurity Behavior in Bulk and Epitaxial $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$," J. Vac. Sci. Technol. B9(3), 1667-1681 (1991).

2. Electron-Longitudinal Optic Mode Scattering

We have studied the Random Element Isodisplacement Model of two-mode behavior. We have also reviewed models for establishing criteria for two mode versus one mode behavior. We have studied effective charges and their meaning for scattering electrons. We have also reviewed the literature. All of these things are discussed in more detail below.

A. Szigeti, Transverse and Callen Effective Charge

Ionic polarizability is caused by the displacements of the ions as a whole while electronic polarizability is caused by the displacement of the electron cloud relative to the nuclei. The displacement of the ions changes the interatomic distance which in turn affects the distribution of the electron cloud. This effect is a short range interaction, since it only depends on the displacement of the near neighbors. There is another type of interaction between atomic and electronic polarizations through the internal field. This effect is a long range effect since the distant dipoles as well as the near dipoles contribute.

Szigeti defined a correction factor s for deviation from heteropolar behavior as a result of mutual distortions of neighboring ions due to their overlapping. Szigeti charge represents the short range interaction of the electronic and atomic displacements. One might expect to find s very different from one if the ions penetrate considerably into each other or if the bond has partial homopolar character and its polarity changes rapidly with the distance between the atoms. Szigeti has shown in his paper how the factor s can be obtained in terms of values that can all be experimentally measured.

The transverse charge is defined to give the local polarization (electronic and atomic) caused by relative displacements. The polarization includes that due to ionic motion and that induced in the electronic charges in the absence of electric fields. The resulting field which scatters electrons is accounted for by separately dividing by ϵ_0 (giving rise to the definition of the Callen charge).

SUMMARY

e_s : The Szigeti Charge $e_s = se$

This is the effective charge used in figuring the force on an ion. Its value is affected by distortion due to overlap. It is a measure of deviation from ideal heteropolar behavior.

e_T : The Transverse Effective Charge
$$e_T = \frac{\epsilon_\infty + 2}{3} e_s$$

This is defined so as to give local polarization induced by relative displacement. We are interested in induced polarization in the absence of electric fields.

e_c : The Callen Effective Charge
$$e_c = e_T/\epsilon_\infty = \frac{\epsilon_\infty + 2}{3\epsilon_\infty} e_s$$

Note for rigid ions $\epsilon_\infty = 1$ and $e_c = e_T = e_s$.

B. One and Two Mode Behavior

In binary alloy systems, lattice vibration spectra can show two different behaviors. The first is "one mode behavior" in which the phonon frequency changes continuously from the value that corresponds to one end member to that of the other end member with an approximately constant strength. The second is "two mode behavior" in which two frequencies occur with a strength approximately equal to the fractional composition of each component.

Experimentally, this behavior can be seen through infrared and Raman spectroscopy. A Kramers-Kronig dispersion analysis can be applied to reflection spectra to get the real part of the dielectric constant $\text{Re } \epsilon(\omega)$, the imaginary part of the dielectric constant $\text{Im } \epsilon(\omega)$, and the imaginary part of the reciprocal of the dielectric constant $-\text{Im } (1/\epsilon(\omega))$. From these functions the frequencies of the transverse optical phonons (TO) and those of longitudinal optical phonons are determined (LO). The frequencies of the TO phonons are determined from the positions of the maxima of the $\text{Im } \epsilon(\omega)$ curve and the frequencies of the LO phonons from the positions of maxima of $-\text{Im } (1/\epsilon(\omega))$ or from the points where the $\text{Re } \epsilon(\omega)$ curve crosses the ω - axis [8]. In the case of the two mode behavior, the Kramer-Kronig analysis yields for each x - value two frequencies of the transverse optical phonons (TO_1 and TO_2) and two frequencies of the longitudinal optical phonons (LO_1 and LO_2).

C. Phenomenological Models Used to Describe Frequency Variation in Mixed Crystal Systems:

- i. Virtual crystal: used to treat "one mode behavior" [1,2]. In this model all masses and spring constants are taken as averages weighted by the mixed crystal composition.
- ii. Cluster model: Verleur and Barker [3], have accounted for the two mode behavior in some mixed crystals using a model based on short range clustering.
- iii. Random Element Isodisplacement (REI) model: the REI model which was proposed by Chen [4] and developed by Chang and Mitra [9] and also by Harada and Narita [10] who assume that in the mixed crystal $AB_{1-x}C_x$ a fraction, $1-x$ of the immediate neighbors of the A-ions are B-ions, and a fraction, x , are C-ions. The B ions and C ions always have A-ions as nearest neighbors. It also assumed that the atoms of the same kind are displaced from equilibrium in the same phase and with the same amplitude. Many details about the application of this model to compound semiconductors to calculate $\omega(x)$ is given in reference [8]. It was shown in reference [11] that with the experimental data for $(\omega(x))$ the two mode behavior in $Hg_{1-x}Cd_xTe$ agrees very well with the theoretical calculations using the REI model. In [10] the reflectivity experimental data were compared to the theoretical one using the REI model. Genzel et al. [12], presented a model completely defined by the macroscopic parameters of the pure end members. They adopted a type of REI model taking into consideration only nearest neighbor interaction.
- iv. Linear chain model [17]: this model was suggested to be the best one [5] for providing a criterion for determination in advance if a mixed crystal will have one or two mode behavior [5]. In this model only nearest neighbor force constants are considered. Mazur et al. [6], have discussed the kind of impurity modes occurring as a result of isotopic substitution in either constituent. This substitution is characterized in terms of a term ϵ defined as

$$\epsilon = 1 - \frac{M'}{M}$$

If $M' < M$, then $1 > \epsilon > 0$ whereas if $M' > M$, $\epsilon < 0$. The results of the impurity mode calculation are given in ref. 6. In substituting for the lighter mass m , a lighter impurity ($\epsilon > 0$) we get a localized mode which rises out of the top of the optical band and for a heavier impurity ($\epsilon < 0$) we get an optical branch gap mode that falls out of the bottom of the same optical branch. In the case of substituting for the heavier mass, if we substitute with a lighter mass ($\epsilon > 0$), we get two modes, a local mode rising out of the top of the optical branch and a gap mode rising out of the top of the acoustical branch. When substituting with a heavier impurity ($\epsilon < 0$) for the heavier mass, no new gap or localized modes are generated. According to the study done by Lucovsky et al. [5], two-mode behavior would be observed in the crystal $AB_{1-x}C_x$ (with $m_c > m_b$) if the substitution of C for B in AB produces a gap mode and if the substitution of B for C in AC produced a localized mode. For a one-dimensional chain, these local and gap modes will occur if A is heavier than B, provided that the lighter end member compound AB has a gap in its phonon spectrum between the optical and acoustic branches. This criteria is applied for MCT and MZT. Although experimentally both MCT and MZT show two mode behavior only MZT seems to meet simple theoretical criteria for such behavior.

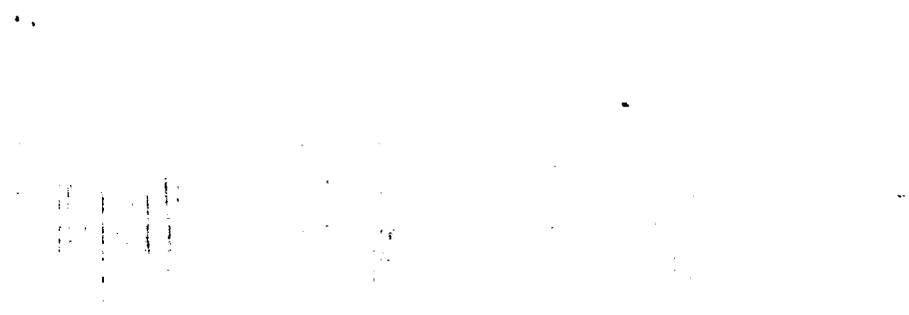
Some experimental data on far-infrared reflection spectra for $Hg_{1-x}Zn_xTe$ are given in reference [13]. Reflectivity data on $Hg_{1-x}Cd_xTe$ are given on reference [14]. In reference [15] calculated values of the optical phonon frequencies as function of composition for $Hg_{1-x}Zn_xTe$ and $Hg_{1-x}Cd_xTe$ using REI model are given and compared with the experimental values. Also the parameters needed for fitting the REI model with the experiment for both materials are given in this paper.

REFERENCES

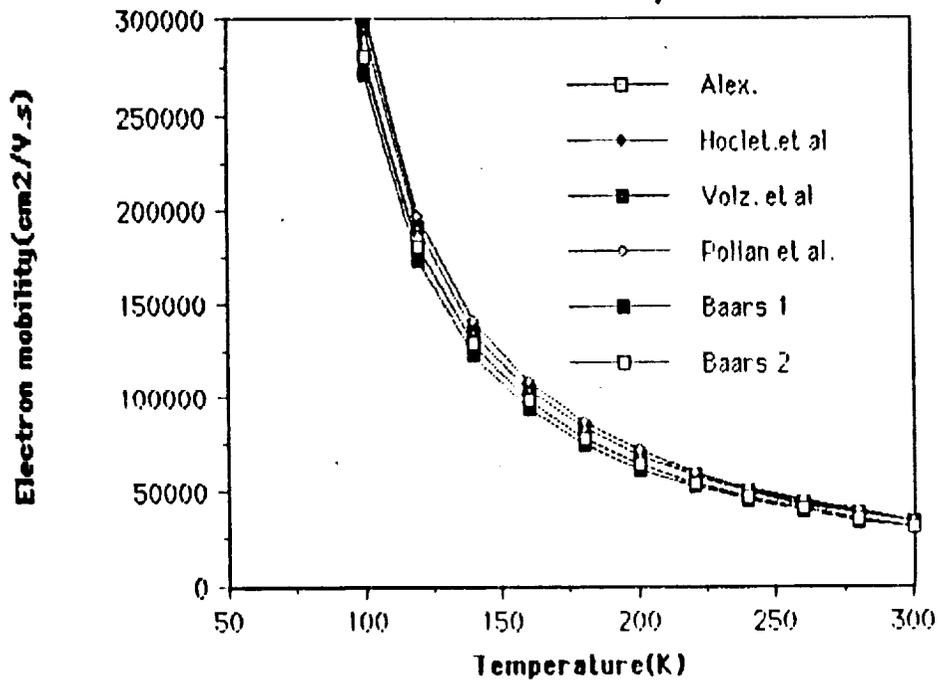
1. J.S. Langer, J. Math. Phys. 2, 584 (1961).
2. Hin-Chiu Poon and A. Bienenstock, Phys. Rev. 147, 710 (1966) and Phys. Rev. 142, 466 (1966).
3. H.W. Verleur and A.S. Barker, Jr., Phys. Rev. 149, 715 (1966).
4. Y.S. Chen, W. Shockley and G.L. Pearson, Phys. Rev. 151 648 (1966).
5. G. Lucovsky, M.H. Brodsky, and E. Burstein, in Localized Excitation in solids, edited by R.F. Wallis (Plenum, New York 1968) p. 592.
6. P. Mazur, E. Montroll and R.B. Potts, J. Wash. Acad. Sci. 46, (1956).
7. F. Matossi, J. Chem. Phys. 19, 161 (1951).
8. M. Gorska and W. Nazarewicz, phys. stat. sol. (b) 65, 193 (1974).
9. I.F. Chang and S.S. Mitra, Phys. Rev. 172, 924 (1968).
10. H. Harada and S. Narita, J. Phys. Soc. Japan 30, 1628 (1971).
11. M. Hoclet, P. Plumelle, M. Vandevyver, R. Triboulet, and Y. Marfaing, phys. stat. sol. (b) 92, 545 (1979).
12. L. Genzel, T.P. Martin, and C.H. Perry, phys. stat. sol. (b) 62, 83 (1974).
13. W. Gebicki, A. Krol. and W. Nazarewicz, phys. stat. sol. (b) 67, K89 (1975).
14. J. Baars and F. Sorger, Solid State Communications, Vol. 10, pp. 875-878, 1972.

15. I.F. Chang and S.S. Mitra, "Long Wavelength Optical Phonons in Mixed Crystals," *Adv. Phys.* 20, 359-404 (1971).

In the following graph we plot mobility versus temperature for several different values of transverse charge which have appeared in the literature. The main difference appears at intermediate temperature where variations of 10% or so can be seen. See also the accompanying table where numbers and references to the values of transverse charge are given.



Effect of using different values of transverse charge on electron mobility



Temp.	Alex.	Hoclet et al	Volz. et al	Polian et al.	Baars 1	Baars 2	
1	60.000	751076.988	784033.540	784824.112	779743.921	745762.683	751620.406
2	80.000	474669.724	493102.113	494049.558	504562.754	465220.325	475571.316
3	100.000	281514.659	295403.722	296080.181	304674.154	271577.235	280418.237
4	120.000	180222.338	190577.704	191046.739	197450.278	173138.017	180278.574
5	140.000	128833.736	135450.259	135788.053	141634.843	122946.166	128853.993
6	160.000	98241.851	104473.185	104729.670	108572.000	94170.610	98234.536
7	180.000	77950.747	83773.962	83976.153	87068.487	75207.492	77915.401
8	200.000	65094.544	69196.174	69359.012	71893.737	62144.293	65077.605
9	220.000	54977.009	58386.936	58520.214	60613.609	52537.899	54960.132
10	240.000	47153.305	50002.296	50112.731	51862.702	45074.538	47137.175
11	260.000	40917.205	43317.087	43406.770	44867.309	39147.968	40902.063
12	280.000	35825.421	37869.652	37947.938	39199.175	34318.862	35812.109
13	300.000	31590.175	33362.540	33429.177	34496.583	30287.202	31578.142
14	320.000	28069.279	29574.540	29636.356	30549.166	26942.153	28058.859
15	340.000	25048.543	26373.168	26422.784	27225.181	24088.784	25039.744
16	360.000	22488.594	23628.672	23673.498	24365.650	21631.696	22480.530

AUTHOR e_T/c (HgTe) e_T/c (CdTe) REFERENCE

Alex	2.96	2.35	S.L. Lehoczky, F.R. Szofran and B.G. Martin, "Advanced Methods for Preparation and Characterization of Infrared Detector Materials, Part 1," NASA CR-161598, Page 70, July 5, 1980.
Hoclet	2.72	2.27	phys. stat. sol (b) 92, 545, (1979)
Volz	2.72	2.239	Solid State Comm., Vol. 75, No. 12, pp. 943-947, 1990
Polian	2.52	2.38	Phys. Rev. B, Vol. 13, Number 8, 1976
Baars	3.2	2.245	Solid State Communic., Vol. 10, pp. 875-878, 1972
Baars	2.981	2.287	Solid State Communic., Vol. 10, pp. 875-878, 1972

used $e_T^* = \frac{\epsilon_\infty + 2}{3} e_s^*$

Reference → Lucovsky et al., Phys. Rev. B, Vol. 4, Number 4, 1367-1371, 1971.

3. Review of Alloy Disorder Scattering

The alloy Hamiltonian can be written, in an approximation, as a uniform virtual crystal Hamiltonian with a residual alloy disorder potential. The alloy disordering scattering typically gives a term proportional to $x(1-x)$. We have not yet studied this in detail, but some relevant references are.

REFERENCES

1. J. Kossut, "The Disorder Scattering in Zincblende Narrow-Gap Semiconduction Mixed Crystals," *phys. stat. sol. (b)* 86, 593 (1978).
2. D.S. Montgomery, "Disorder Scattering and Electron Mobility in $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$," *J. Phys. C: Solid State Physics* 16, 2923-2934 (1983).
3. K.C. Hass, R.J. Lempert, and H. Ehrenreich, "Effects of Chemical and Structural Disorder in Semiconducting Pseudobinary Alloys," *Phys. Rev. Letters* 52, 77-80 (1984).

4. Other Scattering Mechanisms

We have noted that scattering by dislocations may be important but we have not yet examined this in any detail. Zawadski treats scattering by dislocations in the following paper.

REFERENCE

1. W. Zawadski, "Mechanisms of Electron Scattering in Semiconductors," Handbook on Semiconductors Vol. Ch. 12 North-Holland Publ. co. (1982).

5. Further Work on MZT

We should mention that although MZT has several advantages as an IR detector (over MCT) primarily because of its increased Hg stability it also suffers from a greater difficulty in growing uniform crystals. This is because less Zn than Cd is needed for a given E_g

and $\frac{dE_g}{dx}$ for E_g 's of interest is greater for MZT thus small errors in x are magnified in energy gap fluctuations.

Some new papers have appeared. We mention

1. G. Le Bastard, R. Granger, S. Rolland, Y. Marqueton, and R. Triboulet, "Optical Vibration Modes in $Hg_{1-x}Zn_xTe$ Solid Solutions near $q = 0$," J. Phys. France 50 3223-3232 (1989).
2. R. Granger and C.M. Pelletier, "Electron Mobility Evaluation in $Hg_{1-x}Cd_xTe$ and $Hg_{1-x}Zn_xTe$ with Two Mode Optical Dispersion," Presented at 5th Int. Conf. on II-VI Compounds, Yokagama, Japan.
3. R. Granger, A. Lasbley, S. Rolland, C.M. Pelletier, and R. Triboulet, "Carrier Concentration and Transport in $Hg_{1-x}Zn_xTe$ for x near 0.15," J. Crystal Growth 86, 682-688 (1988).
4. S. Rolland, A. Lasbley, A. Seyni, R. Granger, and R. Triboulet, "Electrical Characterization of as-grown, annealed and indium-doped $Hg_{1-x}Zn_xTe$ for x near 0.15," Revue Phys. Appl. 24, 795-802 (1989).
5. E.A. Patten, M.H. Kalisher, G.R. Chapman, J.M. Fulton, C.Y. Huang, P.R. Norton, M. Ray and S. Sen, "HgZnTe for very long wavelength infrared applications," J. Vac. Sci. Technol. B9(3), 1746-1751 (1991).

6. Experimental Data

Good comparisons of our calculations with experimental data have been done in the Ph.D. thesis of Dr. Wafaa A. Gobba. The comparison will be found on the following graph. The abstract of the paper will be found in Section III. Our calculation shows better agreement with experiment than does the calculation of the experimenters. See the following graph.

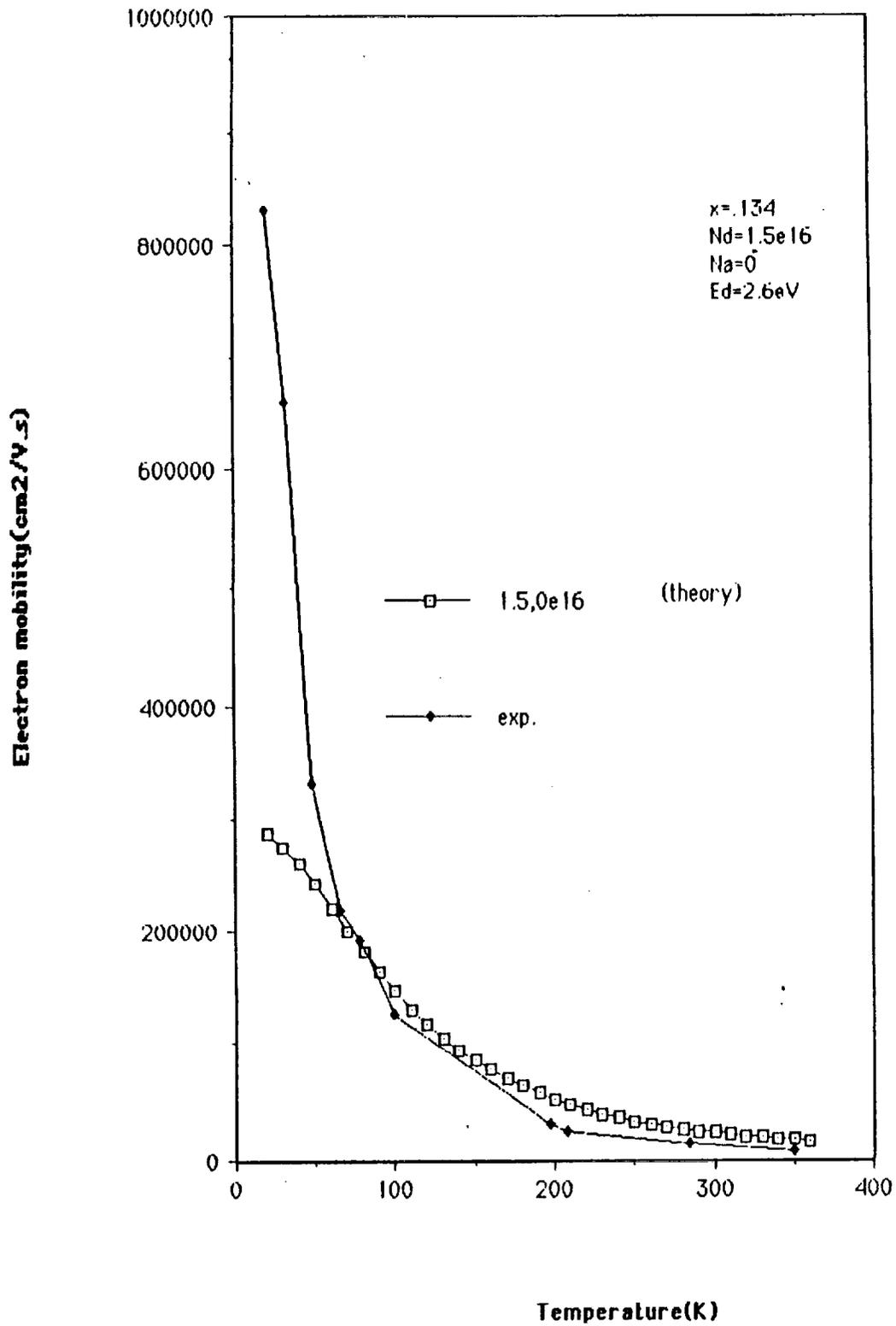


Fig. 7. A comparison between theoretical and experimental results for MZT electron mobility.

7. Superlattices

A superlattice (SL) which has alternating layers of CdTe and HgTe has been proposed by Schulman and McGill as a new IR material which can be made by molecular beam epitaxy. The first successful molecular beam epitaxy growth of a Hg-Te superlatttice occurred in 1982. The band gap depends on the width of the quantum wells as well as the barrier width and height. Thus the formation of HgTe/CdTe superlattices allow a good control of the bandgap which can be a variety from zero to about 1.6 eV. We have also done some rough modeling of high mobility devices which are based on doping in the barrier to furnish electrons to the quantum wells. Some results are given below. Representative references are listed.

There are several comments one could make about the utility of superlattices as IR detectors. In some ways superlattices are an advantage. For one, the energy gap versus SL well layer thickness d_w can be better controlled in SL's than E_g versus x in bulk crystals - at least for E_g 's of interest. This is particularly true because the cut off wavelength for E_g 's of interest is a much more rapidly varying function of x for bulk crystals than of the layer thickness for superlattices.

There exists a neat trick in SL's that can be used to increase the number of electrons without reducing the low temperature mobility due to ionized impurity scattering. This is discussed later. In calculations dealing with electron mobility in superlattices, it has been found that the temperature dependence of the mobility is greatly affected by interface roughness which leads to big complications in making accurate calculations.

There are other advantages to the HgTe-CdTe superlattices as given by Smith, McGill and Schulman. The superlattice tunneling currents are reduced compared to bulk and diffusion currents in photovoltaic devices made from SL's are reduced as is band to band tunneling currents across the junction.

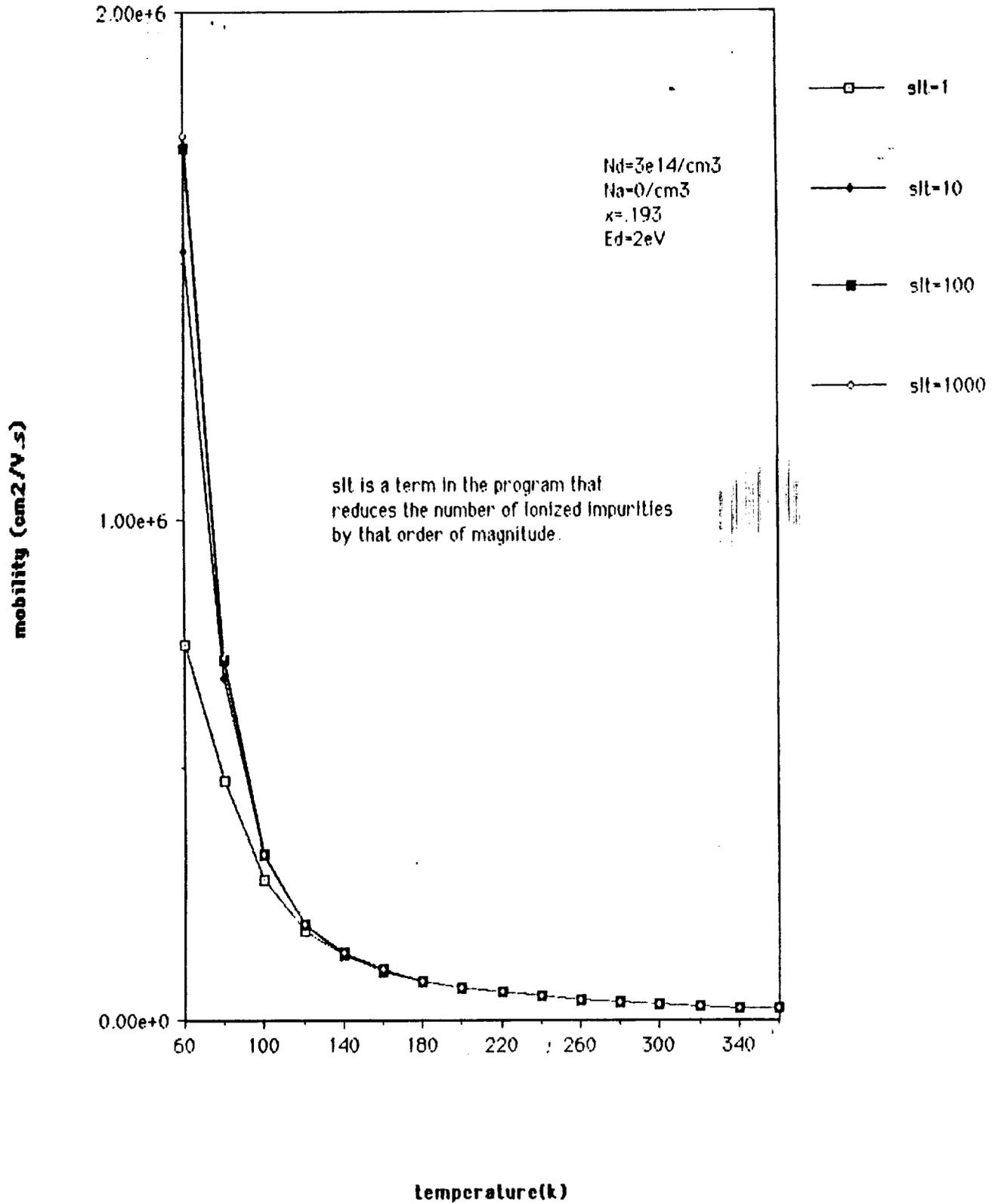
HgTe-ZnTe SL's have also been considered but because of a 6.5% lattice mismatch these become strained layer superlattices. The straining can cause additional effects which may be tailored to advantage.

SELECTED REFERENCES

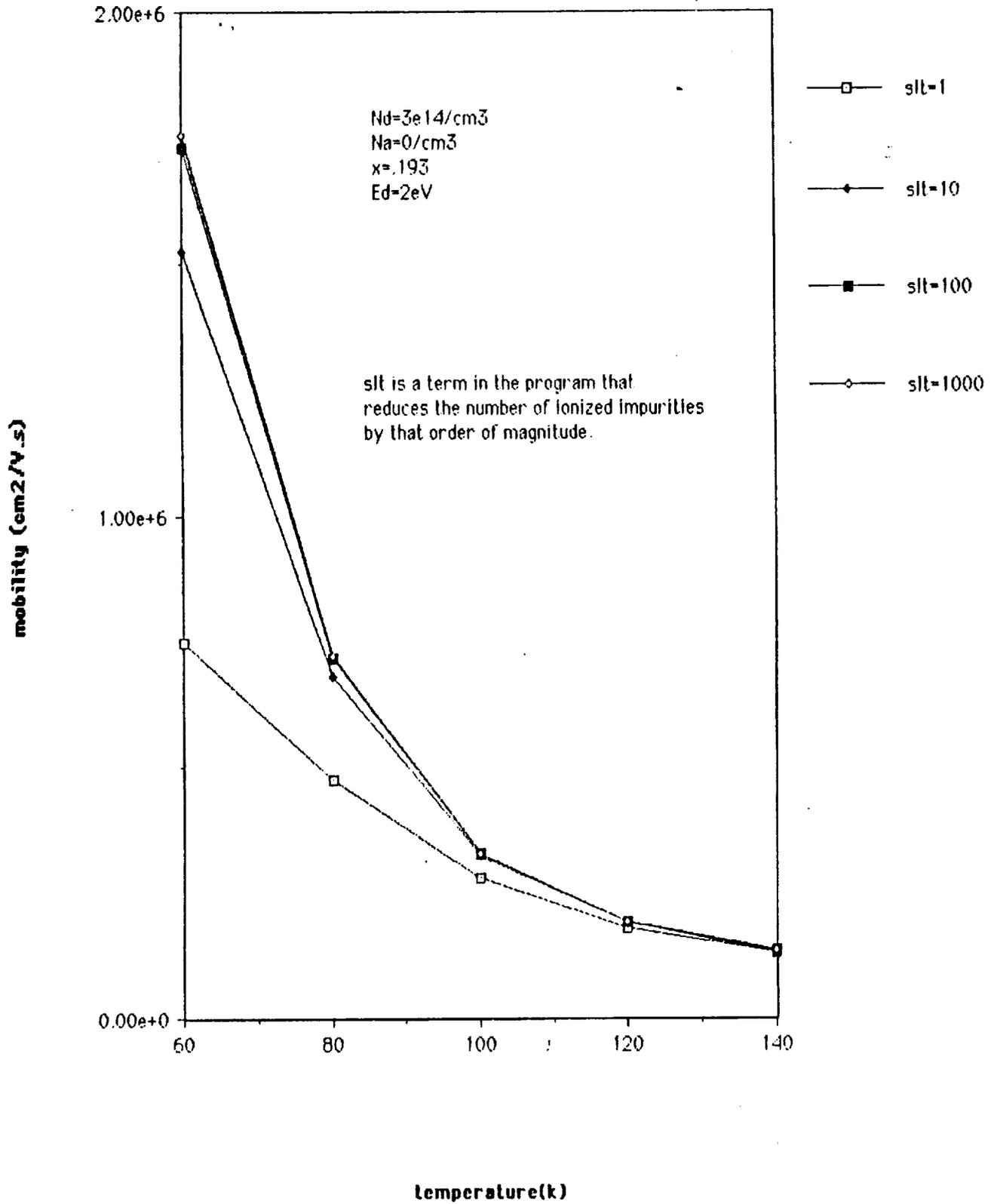
1. J.N. Schulman and T.C. McGill, "The CdTe/HgTe Superlattice: Proposal for a New Infrared Material Appl. Phys. Lett. 34 (10), 663-665 (1979).
2. D.L. Smith, T.C. McGill and J.N. Schulman, "Advantages of the HgTe-CdTe Superlattice as an Infrared Detector Material," Appl. Phys. Lett. 43 (2), 180-182 (1983).
3. Jean-Pierre Faurie, "Growth and Properties of HgTe-CdTe and Other Hg-Based Superlattices," IEEE Journal of Quantum Electronics, Vol. QE-22(9) 1656-1665 (1986).
4. G. Bastard, J.A. Brun, and R. Ferreira, "Electronic States in Semiconductor Heterostructures" in Solid State Physics Editors Henry Ehrenreich and David Turnbull 44, 229-415 (1991).
5. J.R. Meyer, D.J. Arnold, C.A. Hoffman, and F.J. Bartoli, "Theory for Electron and Hole Transport in HgTe-CdTe Superlattices," J. Vac. Sci. Technol. B9(3), 1818-1822 (1991).

In the following graphs we have done a calculation which models very crudely the way that mobility can be enhanced by using layered structures consisting of alternate layers of quantum wells and barriers. If one adds donors in the barriers the resulting electrons will drift to the quantum well resulting in more electrons without more scattering centers. The actual calculation we have done keeps the number of electrons constant and reduces the number of scattering centers. Thus the low temperature mobility (parallel to the layers) would be increased. In the following graphs $sl_t = 10$ means we have N_d electrons at low temperatures with only $N_d/10$ ionized impurities/volume. Further increase of sl_t to 100 produces minimal low temperature gain in the mobility. There is no change in the high temperature mobility reflecting the fact that ionized impurity scattering is not important in this regime. The fact that the effect seems to "saturate" for high electron concentration at low temperature would mean that ii impurity scattering has become negligible due to decrease in ii scattering centers.

A superlattice model for MCT



A superlattice model for MCT



superlatt model

Mon, Nov 25, 1991 3:11 P

	temperat.	sit=1	sit=10	sit=100	sit=1000
1	60.000	751076.988	1525467.598	1733426.082	1757446.805
2	80.000	474669.724	684699.906	719537.439	723240.622
3	100.000	281514.659	323341.664	328613.461	329152.634
4	120.000	180222.338	191148.022	192339.039	192459.921
5	140.000	128833.736	132102.104	132491.781	132530.922
6	160.000	98241.851	99820.114	99981.929	99998.150
7	180.000	77950.747	78686.365	78760.947	78768.415
8	200.000	65094.544	65525.242	65568.739	65573.093
9	220.000	54977.009	55233.843	55259.692	55262.279
10	240.000	47153.305	47316.091	47332.452	47334.089
11	260.000	40917.205	41025.139	41035.974	41037.058
12	280.000	35825.421	35899.483	35906.912	35907.655
13	300.000	31590.175	31642.522	31647.769	31648.293
14	320.000	28069.279	28107.308	28111.118	28111.499
15	340.000	25048.543	25076.820	25079.650	25079.936
16	360.000	22488.594	22509.797	22511.920	22512.132

MCT

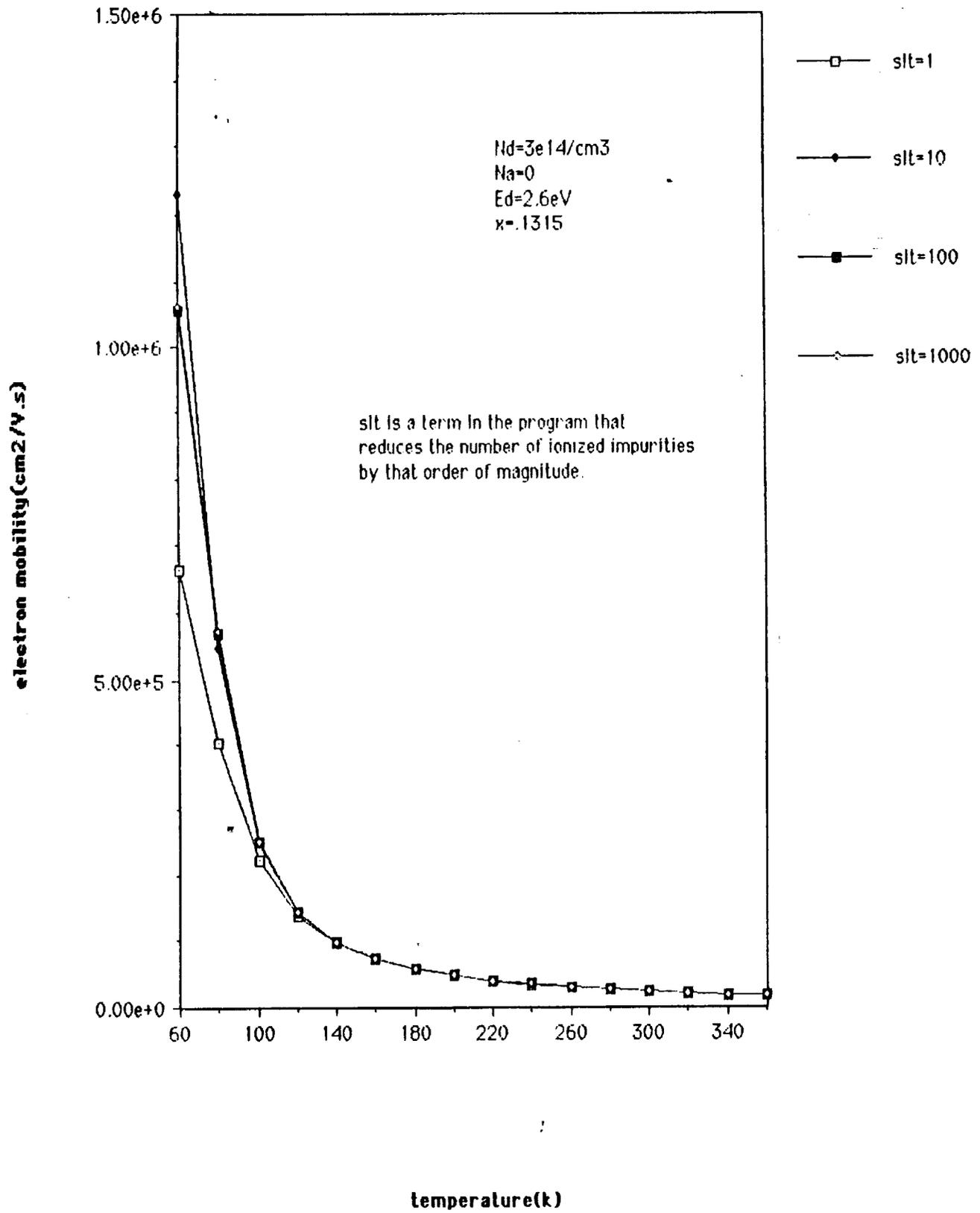
$$N_d = 3 \times 10^{14} / \text{cm}^3$$

$$N_a = 0$$

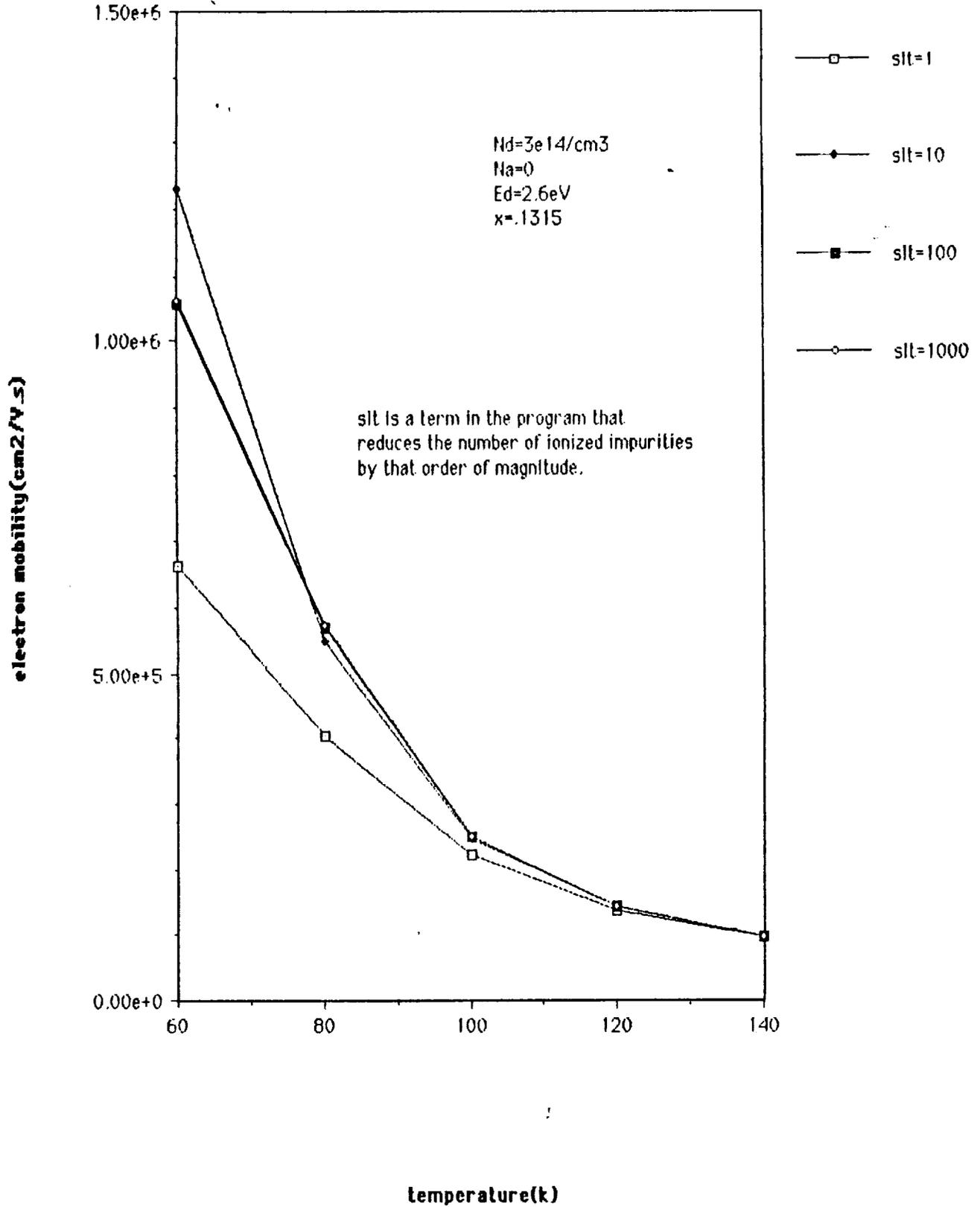
$$E_d = 2 \text{ eV}$$

$$x = 0.193$$

A superlattice model for MZT



A superlattice model for MZT



mzt slit model

Mon, Nov 25, 1991 4:27 PM

	temp.	slit=1	slit=10	slit=100	slit=1000
1	60.000	663572.869	1230497.856	1056335.403	1063633.024
2	80.000	403351.296	547866.320	569450.686	57174.112
3	100.000	222319.312	247811.646	250708.976	251010.634
4	120.000	137639.309	143674.884	144311.660	144375.746
5	140.000	96707.154	98685.643	98889.626	98910.012
6	160.000	73534.903	74362.023	74446.131	74454.687
7	180.000	58764.063	59169.167	59210.093	59214.190
8	200.000	48105.998	48330.619	48351.998	48354.138
9	220.000	40961.376	41093.482	41106.755	41108.083
10	240.000	35135.113	35218.506	35226.873	35227.710
11	260.000	30507.501	30562.866	30568.410	30568.964
12	280.000	26734.495	26772.450	26776.253	26776.634
13	300.000	23611.429	23638.902	23641.592	23641.861
14	320.000	20978.397	20997.839	20999.786	20999.981
15	340.000	18757.040	18771.454	18772.897	18773.042
16	360.000	16854.456	16865.331	16866.419	16866.520

MZT

$$N_d = 3 \times 10^{14} / \text{cm}^3$$

$$N_a = 0$$

$$x = .1315$$

$$E_d = 2.6 \text{ eV}$$

REFERENCES

We have gathered many references in all these areas and they will be summarized in the Final Report.

II. LIST OF REPORTS AND PAPERS

1. W.A. Gobba, "Theoretical Calculations of Electron Mobility in Narrow Gap Semiconductors," Invited talk to be presented at Annual Meeting of Am. Assoc. of Phys. Teachers, Orlando, FL, January 1991.
2. W.A. Gobba, J.D. Patterson and S.L. Lehoczky, "Electron Mobility in Mercury Zinc Telluride Alloys," Talk to be presented at March Meeting of the American Physical Society, Indianapolis, 1992.
3. J.D. Patterson, W.A. Gobba, "Enhanced Screening in Doped Semiconductors," March Meeting of the American Physical Society, Indianapolis, 1992.
4. Wafaa M.K.A. Gobba, "Theory of Electron Mobility in Narrow Gap Semiconductors," Ph.D. Thesis, Florida Institute of Technology, August 1991.
5. J.D. Patterson, Wafaa A. Gobba and S.L. Lehoczky, "Electron Mobility in n-type HgCdTe and HgZnTe Alloys." Revised preprint.

**III. APPENDIX:
ABSTRACTS OF PAPERS, REPORTS, AND TALKS**

Theoretical Calculations of Electron Mobility in Narrow Gap Semiconductors *

WAFAA A. GOBBA, Department of Physics and Space Sciences, Florida Institute of Technology, Melbourne, FL 32901

The prototype narrow gap semiconductor we deal with is Mercury Cadmium Telluride (MCT) because of its applicability to making Infrared (IR) detectors. Interest has focused on $Hg_{1-x}Cd_xTe$ because its band gap is tunable with x , and because it can operate efficiently as an IR detector at 77K in the atmospheric window of wavelength 8-12 microns. We also do calculations on Mercury Zinc Telluride (MZT) and find for equivalent energy gaps that its mobility, as a function of temperature, is similar to MCT. Because of Mercury stability MZT may turn out to be a better IR detector. Our calculations are state of the art and involve the Boltzmann equation, its solution by the variational principle and they include all relevant interactions. The results compare well with experiments. Comments will be made about how the author came to specialize in this area and the opportunities and challenges that exist for women.

* Supported by NASA Contract Number NAG-781.

Suggested title of session
in which paper should be
placed: II - VI Semiconductors

Abstract Submitted
for the Indianapolis Meeting of
the American Physical Society
16-20 March 1999

Physics & Astronomy
Classification Scheme
Number 75.20

Electron Mobility In Mercury Zinc Telluride Alloys. * WAFAA A. GOBBA, J. D. PATTERSON, Dept. of Physics and Space Sciences, F.I.T., and S.L. LEHOCZKY, Marshall Space Flight Center - We have calculated the mobility of electrons in n-type Mercury Zinc Telluride (MZT) and compared it to a calculation of the mobility of electrons in n-type Mercury Cadmium Telluride (MCT) with nearly the same energy gap and with the same number of donors and acceptors. We find for equivalent energy gaps that the mobilities in the two compounds (MCT, MZT) are nearly the same. The calculations for both MCT and MZT are based on the best set of materials parameters that we can compile from the literature, and the MZT compilation is much more complete than was previously available. Since MZT is harder and structurally more stable with respect to Hg retention than MCT, the possibility of equivalent mobility for MCT and MZT is significant. This calculation is one of the first extensive calculations of the mobility of MZT, and we compare it to another by Rolland et al. (Revue Phys. Appl. 24, 795 - 802 (1989)) which appears to be less extensive. Our calculation yields very good results as compared to experiment except at very low temperatures where its accuracy is limited by a lack of knowledge of ionized impurity concentration. Mobilities in the range of 10^5 cm²/vs at 100 K are typical. Our calculation involves scattering of the electrons by longitudinal optic phonons, acoustic phonons, ionized impurities, holes, and compositional disorder. Since not all of these interactions can be approximated by elastic scattering, the corresponding Boltzmann equation is solved by a variational principle. * Supported by NASA Contract No. NAG-781

(X) Prefer Standard Session

James D. Patterson
Signature of APS Member
James D. Patterson
Florida Institute of Technology
Physics/Space Science Dept.
Melbourne, FL 32901

Suggested title of session
in which paper should be
placed: Defects In Semiconductors

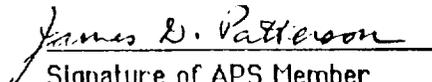
Abstract Submitted
for the Indianapolis Meeting of
the American Physical Society
16-20 March 1992

Physics & Astronomy
Classification Scheme
Number 73.20

Enhanced Screening In Doped Semiconductors.

J.D. PATTERSON and WAFAA A. GOBBA, Dept. of Physics and Space Sciences, Florida Institute of Technology -- Semiconductors with shallow donor centers are considered. The donor energy levels are assumed to be discrete but screened by electrons from the conduction band. High doping levels are assumed. The number (n) of electrons in the conduction band is increased by screening which reduces their binding energy causing the promotion of more electrons to the conduction band and further reducing the binding energy etc. The equations describing this effect are analogous to mean field equations. The effect is temperature dependent and near a certain temperature there can be a rapid increase of n with temperature. The abrupt increase in n is, of course, reminiscent of other abrupt changes related to screening such as the Mott transition. We predict it should be observable for reasonable values of parameters such as in GaAs at $T \cong 20\text{K}$ with 5×10^{16} donors/cm³ and for donor binding energy of 12 meV. Some other aspects of screening in semiconductors will also be discussed.

(x) Prefer Standard Session


Signature of APS Member
James D. Patterson
Florida Institute of Technology
Physics/Space Sciences Dept.
Melbourne, FL 32901

FLORIDA INSTITUTE OF TECHNOLOGY

A dissertation submitted in partial fulfillment
of the requirement for the degree of
Doctor of philosophy
in
Physics

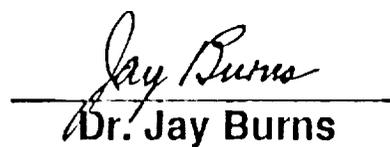
Theory of electron mobility in narrow-gap semiconductors

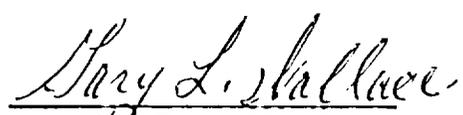
by

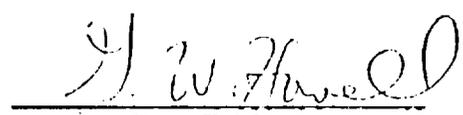
Wafaa M. K. Abdelhakiem Gobba

Approved by :


Dr. J.D. Patterson
Professor and Head
Physics and space sciences


Dr. Jay Burns
Professor
Physics and space sciences


Dr. Gary Wallace
Assistant Professor
Physics and space sciences


Dr. G.W. Howell
Associate Professor
Applied Mathematics

ABSTRACT

The electron mobility, concentration of electrons, light holes and heavy holes, and Fermi energy in n-type $\text{Hg}_{1-x}\text{Zn}_x\text{Te}$ (MZT) have been calculated and compared with those of $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ (MCT) for the same energy gap (but different x), and the same donor and acceptor concentration. The results for MZT were found to be very close to those of MCT. The calculation relied on solving the Boltzman transport equation using variational principles. The processes that were of significance included the scattering of electrons by : ionized impurities, holes, compositional disorder, acoustical phonons and optical phonons. In the process of calculating the results for MZT a table for the latest values of all the needed material parameters was obtained by a literature search.

MZT has been considered as a substitute for MCT for possible use in infrared detectors due to its relative stability and hardness. Our theoretical results for MZT were compared to the experimental results published by Rolland et al. and Granger et al. and very good agreement over most of the temperature range was obtained.

The effect of making changes on some of the relevant parameters in the calculation was checked. Also, adding neutral impurities to the scattering processes and using the most recent published band parameters of MCT (rather than the slightly older values) on the electron calculation did not produce significant changes.

The speed of a very involved and long program has been increased by changing its code from Basic for an HP 9845 to FORTRAN for a Vax 11/780 and later a Sun workstation 386i. This program was given to us by Dr. S. L. Lehoczky and it was written to calculate the electron mobility, the free carrier concentrations, and the Fermi energy for MCT. All of these were calculated as a function of temperature, composition, donor and acceptor concentration. The program was checked, corrected and fine tuned by including the latest values of material parameters for MCT, another version was made to run for MZT and neutral defect scattering was added to the program.

**ELECTRON MOBILITY IN n-TYPE
Hg_{1-x}Cd_xTe AND Hg_{1-x}Zn_xTe ALLOYS***

J.D. Patterson and Wafaa. A. Gobba
Department of Physics and Space Sciences
Florida Institute of Technology
Melbourne, FL 32901-6988 U.S.A.

and

S.L. Lehoczky
ES75, Space Science Laboratory
Marshall Space Flight Center, AL 35812 U.S.A.

ABSTRACT

We have calculated the mobility of electrons in n-type Mercury Cadmium Telluride (MCT) and compared it to a calculation of the mobility of electrons in n-type Mercury Zinc Telluride (MZT) with nearly the same energy gap and with the same number of donors and acceptors. We also compared the results of the MZT calculation with experiment. We found for equivalent energy gaps that the mobilities in the two compounds (MCT, MZT) were nearly the same. The calculations for both MCT and MZT were based on the best set of material parameters that we could compile from the literature. Using these parameters, the comparison with experiment for MZT yielded very good results. Since MZT is harder and structurally more stable with respect to Hg retention than MCT, the possibility of equivalent mobility for MCT and MZT is significant.

This calculation is one of the first extensive calculations of the mobility of MZT, and we compared it to another which appeared to be less extensive. Our calculation involves scattering of the electrons by longitudinal optic phonons, acoustic phonons, ionized impurities, holes, and compositional disorder. Since not all of these interactions can be approximated by elastic scattering, the corresponding Boltzmann equation was solved by a variational principle. We also discuss directions for future work.