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FINAL REPORT

TITLE OF GRANT:

IMPROVEMENT OF PROGRAM TO CALCULATE ELECTRONIC
PROPERTIES OF NARROW BAND GAP MATERIALS

TYPE OF REPORT:

BRIEF SUMMARY OF ENTIRE PROJECT

NAME OF PRINCIPAL INVESTIGATOR:

JAMES D. PATTERSON

PERIOD COVERED BY THE REPORT:

JUNE 15, 1989 TO JUNE 15, 1991
(INCLUDING 1 YEAR NO COST EXTENSION)

NAME AND ADDRESS OF THE GRANTEE INSTITUTION:

FLORIDA INSTITUTE OF TECHNOLOGY
150 W. UNIVERSITY BOULEVARD
MELBOURNE, FL 32901-6988

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GEORGE C. MARSHALL SPACE FLIGHT CENTER
MARSHALL SPACE FLIGHT CENTER, AL 35812
(TECHNICAL OFFICER SANDOR L. LEHOCZKY, ES75)

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We acknowledge the support of NASA for this work. Our contract monitors at Marshall Space Flight Center, Dr. Sandor L. Lehoczky and Gretchen L. Perry have been very supportive. We also appreciate the support and facilities made available to us at the Florida Institute of Technology, both in the Space Research Institute and in the Physics and Space Science Department, especially the word processing of Elaine Hooker.

BRIEF SUMMARY OF

"Improvement of Program to Calculate Electronic Properties of Narrow Gap Materials"

- I. Listing of tasks accomplished
- II. List of reports and papers
- III. Appendix: Abstracts and other documentation related to reports and papers
 - A. "A Comparison Between Electron Mobility in n-type $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ and $\text{Hg}_{1-x}\text{Zn}_x\text{Te}$."
 - B. Abstract from "Electron Mobility in n-type $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ and $\text{Hg}_{1-x}\text{Zn}_x\text{Te}$ Alloys."
 - C. Introduction to "The Effects of Screening on the Scattering of Electrons by Neutral Defects."
 - D. Abstract for Report "Improvement of Program to Calculate Electronic Properties of Narrow Band Gap Materials."
 - E. Abstract for Grant Proposal "Further Improvement in Program to Calculate Electronic Properties of Narrow Band Gap Materials."
 - F. Outline for talk on Electron Mobility in Narrow Gap Semiconductors.

I. LISTING OF TASKS ACCOMPLISHED

- A. The program has been sped up by reprogramming it so it will run on both a SUN and a VAX. Also it is easily transportable as we have it on a disk for use on a SUN (See II D).
- B. We have made a computer literature search and have compiled a reference list. The search has resulted in some improved parameters for $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ and a table of parameters for $\text{Hg}_{1-x}\text{Zn}_x\text{Te}$ (See II D).
- C. We have added the effects of neutral defects to the program and found, as expected, that they contribute very little to the mobility at temperatures of interest (See II D).
- D. We have added the effects of varying the following parameters (See II D).
 - 1. Dielectric Constants
 - 2. Screening Parameters
 - 3. Disorder Energies
 - 4. Donor and Acceptor Concentrations
 - 5. Momentum Matrix Element
 - 6. Different Expressions for Energy Gap
 - 7. Transverse Effective Charge
- E. A new grant proposal "Further Improvement in Program to Calculate Electronic Properties of Narrow Band Gap Materials" has been submitted to MSFC. An abstract of this is enclosed in the Appendix E.
- F. A talk on this work has been prepared and presented at various seminars. An outline is enclosed in Appendix F.

II. LIST OF REPORTS AND PAPERS

- A. The following paper has been published. "A Comparison Between Electron Mobility in n-type $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ and $\text{Hg}_{1-x}\text{Zn}_x\text{Te}$," by W. Abdelhakiem, J.D. Patterson and S.L. Lehoczky. *Materials Letters* 11, 47-51 (April 1991). It is included in Appendix A.
- B. A longer paper "Electron Mobility in n-type $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ and $\text{Hg}_{1-x}\text{Zn}_x\text{Te}$ " is being revised by adding comparison to experimental results. The abstract is included in Appendix B. An initial copy has been sent to Technical Officer S.L. Lehoczky.
- C. A short paper "The Effects of Screening on the Scattering of Electrons by Neutral Defects" has been submitted to *physica status solidi b*. The introduction to this article is included in Appendix C. An initial copy has been sent to Technical Officer S.L. Lehoczky.
- D. A very long comprehensive report "Improvement of Program to Calculate Electronic Properties of Narrow Band Gap Materials" has been prepared. It is too long for publication but a corrected copy has been sent to S.L. Lehoczky--the Technical Officer for this proposal. An abstract is included in Appendix D.

APPENDICES

A. A Comparison between electron mobility in n-type $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ and $\text{Hg}_{1-x}\text{Zn}_x\text{Te}^*$

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Abstract

We have calculated the electron mobility in n-type $\text{Hg}_{1-x}\text{Zn}_x\text{Te}$ (MZT) and compared it with that of $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ (MCT) for the same energy gap, donor concentration and acceptor concentration. The calculated MZT electron mobility was found to be very close to MCT electron mobility. For our calculations, we solved the Boltzmann equation using variational principles. The scattering processes that are of significance for our calculations include the scattering of electrons by : ionized impurities, holes, compositional disorder, acoustic phonons and optical phonons. In the process of calculating the electron mobility for MZT we have set up a table for all the needed material parameters. MZT has been considered as a substitute for MCT for possible use in infrared detectors due to its relative stability and hardness .

Introduction

$\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ (MCT) is a very useful material for Infrared detectors because it has a large carrier mobility at liquid nitrogen temperature and its energy gap allows, for suitable x , absorption in the two atmospheric windows (3-5 μm and 8-14 μm). For this reason scientists have done a large amount of research on MCT, studying for example, its band structure and transport properties.

Unfortunately the CdTe bond [1] destabilizes the weak HgTe bond in MCT alloys leading to lattice, surface and interface [2,3] instabilities. At the same time HgTe is stabilized by alloying it with ZnTe. It has also been shown that MZT ($\text{Hg}_{1-x}\text{Zn}_x\text{Te}$) is a harder material than MCT due to the fact that the ZnTe bond length (2.406Å) is shorter than that of HgTe (2.797Å) or CdTe (2.804Å) [1].

By calculating the electron mobility of n-type HgZnTe and comparing it with that of HgCdTe for the same energy gap as well as the same donor and acceptor concentration, we found that the electron mobilities are very close.

This makes MZT a better material to be used for Infrared photodetection because it has the same band structure and is more stable and much harder than MCT.

Theory

The theory here is much more complicated than the theory of simple semiconductors. These complications arise due to the nonparabolicity of the energy band and the high ionicity of the material which makes the polar interaction of the electrons with the longitudinal phonons play an important role at high temperature. In this interaction, the phonon energy is comparable to the electron energy. The scattering is inelastic, the relaxation time approximation is inappropriate and the variational principle has to be used to solve the Boltzmann equation. Another complication is due to narrowness of the band gap which implies a non-negligible number of thermally excited electrons and so screening has to be taken into consideration.

Explicitly, the collision processes considered in our calculations are: ionized impurities, holes, compositional disorder, acoustic phonons and optical phonons. Neutral defect scattering, at reasonable concentrations, did not cause any significant changes in electron mobility calculations. At low temperature for n-type materials, the scattering is mainly due to ionized impurities. This scattering process decreases with increasing temperature since the charged impurity atoms do not scatter high energy electrons. The theory

for hole scattering is somewhat similar to ionized impurities. At high temperature, the scattering is mainly due to longitudinal optical phonons. Since the two atoms in the unit cell are different, the longitudinal optical mode of the lattice vibrations polarizes the crystal and an electric field is produced. The Frolich perturbation potential is used to describe the interaction of the electrons with that field. For the acoustic phonons we use the deformation potential which arises from the changes in the energy band gap which is a result of the changes in the spacing of the lattice atoms. In a compound semiconductor, like HgCdTe electrons suffer an additional scattering due to the random location of Hg and Cd. This is the compositional disorder scattering.

Thus by knowing the band model of the compound semiconductor, finding the needed material parameters from the published experimental work, studying all the significant scattering processes, knowing the corresponding potential for each scattering, calculating the scattering matrix element, setting up the Boltzman equation and solving it using variational principles, we calculated the electron mobility for MCT and MZT.

Results and discussion

First, we calculated and plotted the values of the energy gap, concentration of electrons in the conduction band, concentration of light and heavy holes versus temperature for both alloys over a range from 60K to 360K. These results are shown in Fig.1[a-d]. The concentration of the carriers is very close since the small difference in the carrier concentration at higher temperature is due to the small difference in the energy gap for the same temperature range.

In our calculations we used $N_d = 3 \times 10^{14} / \text{cm}^3$, $N_a = 0 / \text{cm}^3$, $x(\text{MZT}) = .1315$, $x(\text{MCT}) = .193$, $E_D(\text{MCT}) = 2\text{eV}$, $E_D(\text{MZT}) = 2.6\text{eV}$ and $\Delta(\text{MZT}) = 1.0\text{eV}$. For MCT, the parameters we used were those values given by Lehoczky et al. [14]. For MZT we evaluated and collected all the needed parameters from the literature and they are given in Table [1]. See also comments [a-d] listed at the end of the references and referred to by table [1].

Two kinds of donors were used in the analysis. The first one had a donor level coinciding with the conduction band minimum and so was assumed to be fully ionized. Its density was determined by assuming $N_d - N_a$ to be equal to the electron concentration at very low temperature. The second kind was used to explain the temperature dependence of the electron concentration below 80K

for a particular sample. The ionization energy of states and their densities are determined by fitting the data given in reference [14]. We just used these values as typical and thus in our model we used 1meV for the ionization energy and $10^{14}/\text{cm}^3$ for the density. For this concentration of bound donors, only at low temperature was there any effect on the mobility and it was small. We then compared, see Fig.[2], the electron mobility in n-type MCT and MZT, and they came out to be very close at all temperatures when the energy gap and the donor and acceptor concentration were the same. We also evaluated the electron mobility for different donor and acceptor concentration with the same net carrier concentration ($N_d = 5 \times 10^{14}/\text{cm}^3$, $N_a = 2 \times 10^{14}/\text{cm}^3$, $x(\text{MZT}) = .1315$, $x(\text{MCT}) = .193$) and got similar results.

Unfortunately, there has not been any published data for the electron mobility in n-type well characterized bulk materials of MZT that we can compare our results to. Some thin film data is available [20,21] but it is not directly comparable. However, this type of calculation has been done for MCT and compared with the experimental values in reference [17], where reasonable agreement was achieved for bulk materials.

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a) E_I was calculated using hydrogenic approximation [16].

b) $\rho(\text{ZnTe}) = 5.636 \text{ gm/cm}^3$ [9], $\rho(\text{HgTe}) = 8 \text{ gm/cm}^3$ [16], $c_{11}(\text{ZnTe}) = 7.13$ [9]

$c_{11}(\text{HgTe}) = 5.08$, $c_{44}(\text{ZnTe}) = 3.12$, $c_{44}(\text{HgTe}) = 2.05$ [10]

$v_l = \sqrt{\frac{c_{11}}{\rho}}$, $v_t = \sqrt{\frac{c_{44}}{\rho}}$ [16], (These two equations gave the values of v_l and v_t

at the end points. For the intermediate points we used a linear interpolation.)

c) Due to lack of published data, the low frequency dielectric function of

$\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ was used, where it has the right value at $x=0$ and was off by 2% at $x=1$.

d) The disorder energy for $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ is 1.85 eV [17].

Since $E_g(\text{CdTe}) = 1.59 \text{ eV}$ [18] then if $z = E_g(\text{HgTe})$ we have for the disorder energy (equal to the difference in bandgap energies):

$$E_d(\text{MCT}) = 1.59 - z = 1.85, \text{ so } z = -.26 \text{ eV}$$

For MZT Berding [18] gives $E_g(\text{ZnTe}) = 2.37 \text{ eV}$

so $E_d(\text{MZT}) = 2.37 + .26 = 2.63 \text{ eV}$. These are really low temperature results, but for convenience we use them at all temperatures.

Table 1. Parameters for electron mobility and charge carrier concentration calculations for $\text{Hg}_{1-x}\text{Zn}_x\text{Te}$

Parameter	Value	Reference
Spin orbit splitting	$\Delta = 0.9 \text{ eV}$	(4)
	$\Delta = 1.0 \text{ eV}$	(5)
Heavy hole mass	$m_{hh} = 0.6 m_0$	(5)
Acoustic deformation potentials (a)	$E_0 = 9.5 \text{ eV}$ Longitudinal mode	(6)
	$E_1 = 4 \text{ eV}$ Transverse mode	(7)
	$E_2 = 3 \text{ eV}$ Transverse mode	(8)
Longitudinal sound velocity (b)	$v_L = (2.52 + 1.037x) \times 10^5 \text{ cm/sec}$	(9),(10),
Transverse sound velocity (b)	$v_T = (1.6 + 0.753x) \times 10^5 \text{ cm/sec}$	(16)
Hg mass	$m_{\text{Hg}} = 200.59 \text{ a.m.u}$	
Zn mass	$m_{\text{Zn}} = 65.37 \text{ a.m.u}$	
Te mass	$m_{\text{Te}} = 127.6 \text{ a.m.u}$	
Lattice constant	$a_0 = (6.451 - 0.2857x) \text{ \AA}$	(11)
$\Gamma_6 - \Gamma_8$ Energy gap	$E_g(x,T) = -0.3 + 3.24 \times 10^{-2} x^{1/2} + 2.731x - 0.629x^2 + 0.533x^3 + 5.3 \times 10^{-4} T(1 - 0.76x^{1/2} - 1.29x)$ $0.1 \leq x \leq 0.4, 50 \leq T \leq 350$	(5)
Momentum matrix element coupling conduction and valence bands.	$P = 8.2 \times 10^{-8} \text{ eVcm}$	(5)
Transverse effective charges	HgTe $e_T/e = 2.96$	(7)
	ZnTe $e_T/e = 2.0$ Experimental $= 1.86$ Theoretical	(12)
Reduced mass	$m_{\text{HgTe}} = 1.295 \times 10^{-22} \text{ g}$ $m_{\text{ZnTe}} = 7.178027 \times 10^{-23} \text{ g}$	
Dielectric constants (c)	$\epsilon_0 = 20.206 - 15.153x + 6.59091x^2 - 0.951826x^3$	(6),(14), (15),(16)
	$\epsilon_\infty = 13.2 - 19.1916x + 19.7496x^2 - 6.458x^3$	(19)
HgTe Lo phonon frequency	$\omega_{\text{LoHgTe}} = (135 + 19x - 18x^2) \text{ cm}^{-1}$	(13),
HgTe To phonon frequency	$\omega_{\text{ToHgTe}} = (118 + 34x - 16x^2) \text{ cm}^{-1}$	(16),
ZnTe Lo phonon frequency	$\omega_{\text{LoZnTe}} = (165 + 44x) \text{ cm}^{-1}$	(19)
ZnTe To phonon frequency	$\omega_{\text{ToZnTe}} = (165 + 12x) \text{ cm}^{-1}$	
Disorder energy (d)	2.6 eV	(17),(18)

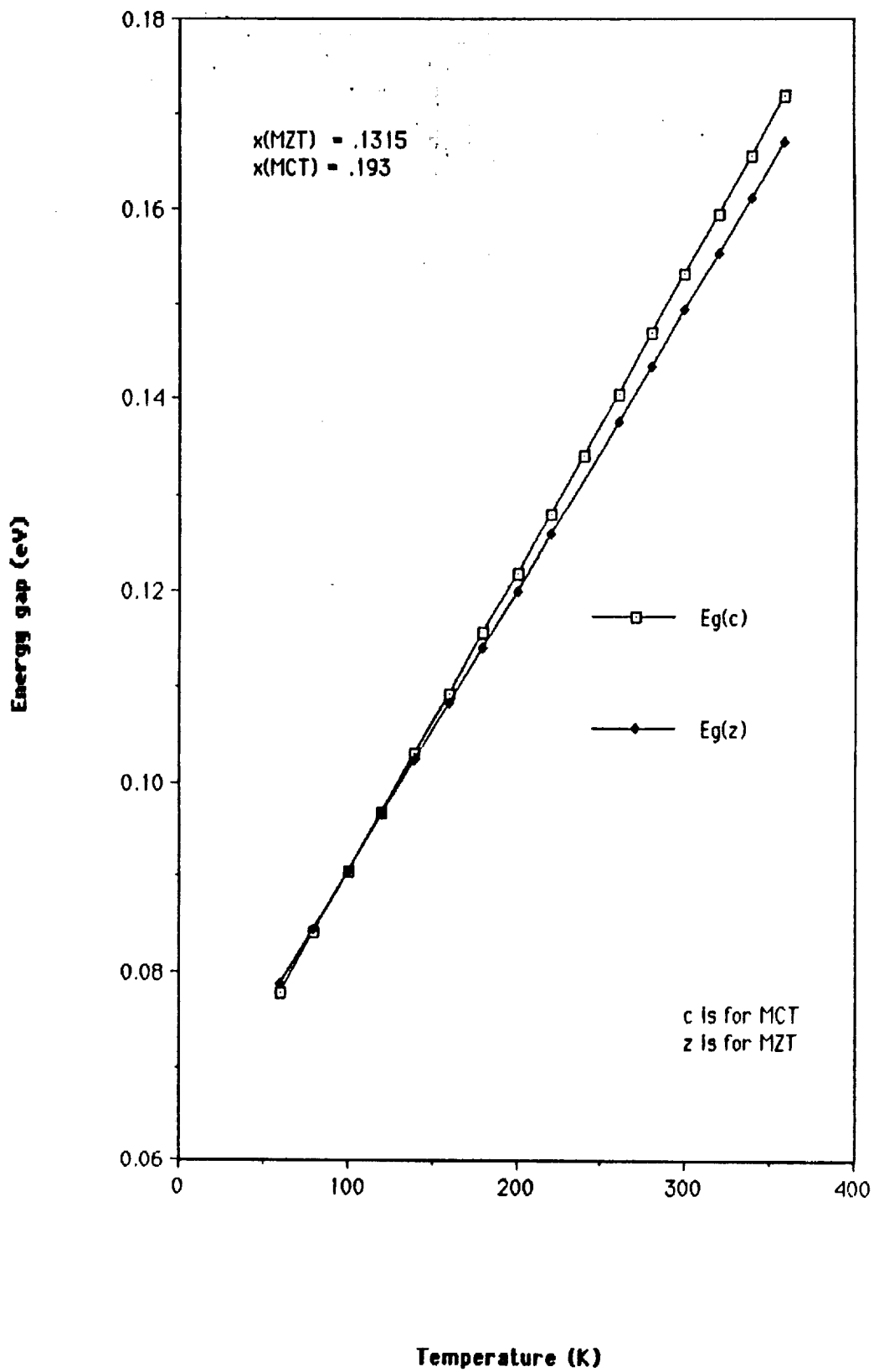


Fig.1a

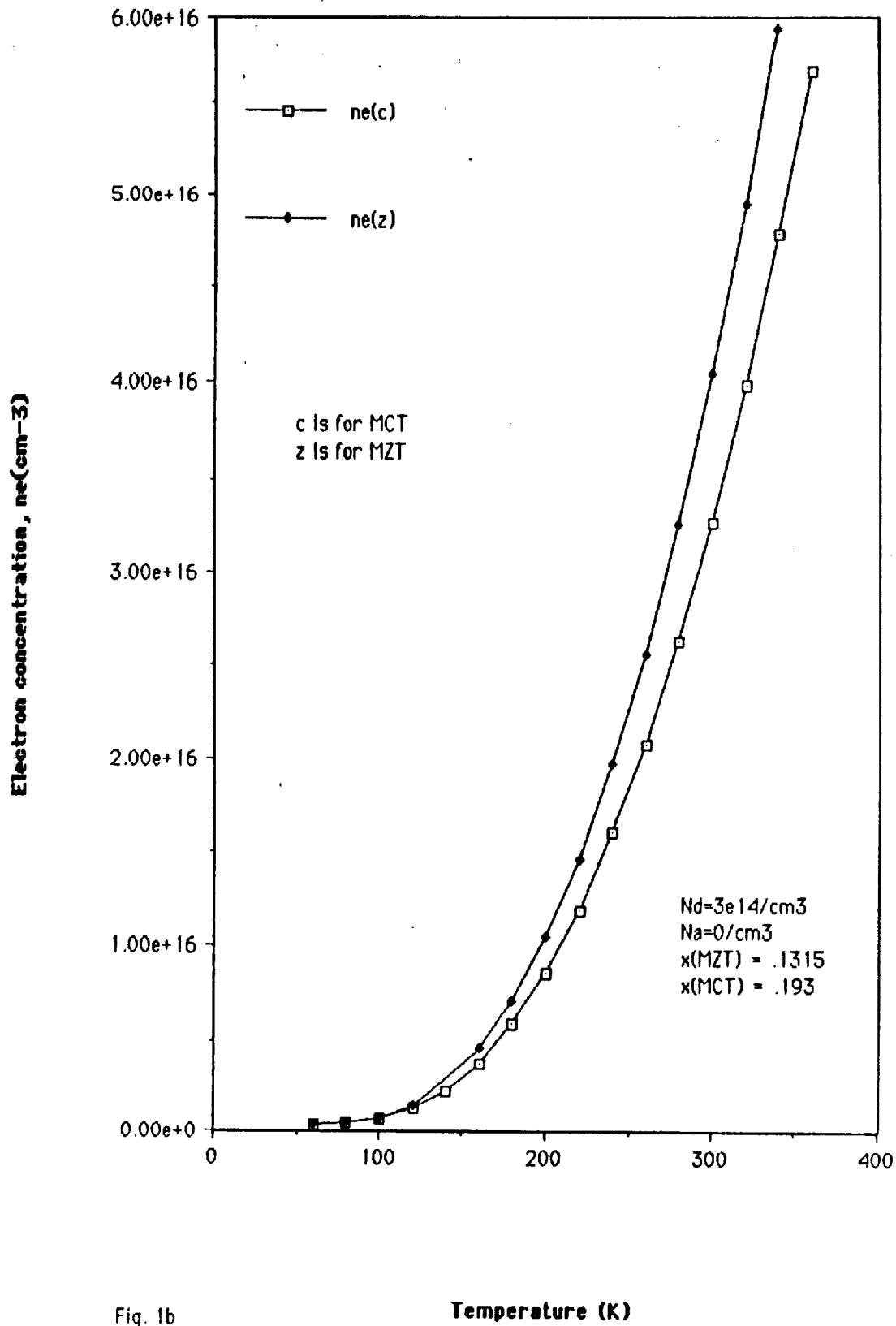


Fig. 1b

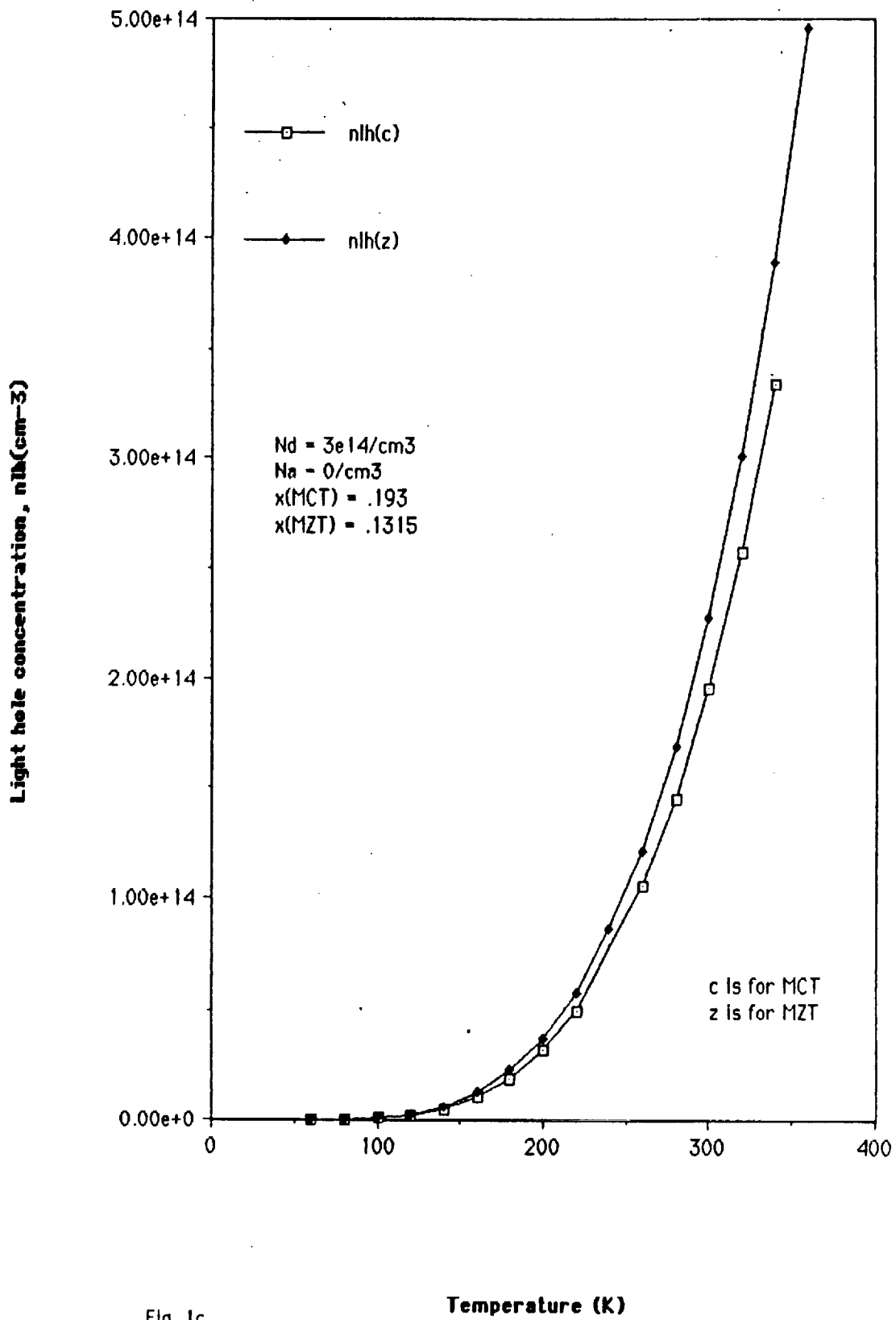


Fig. 1c

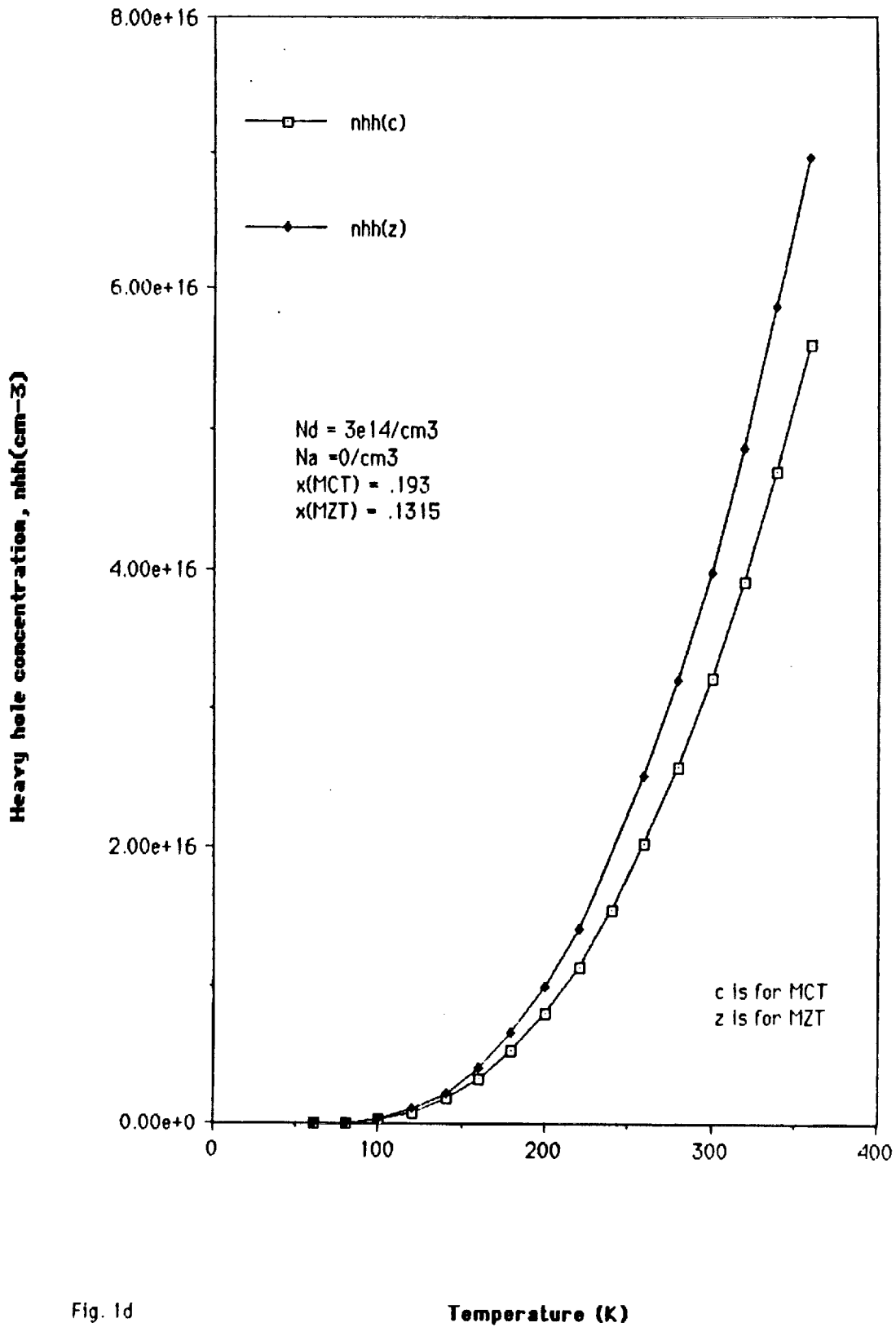


Fig. 1d

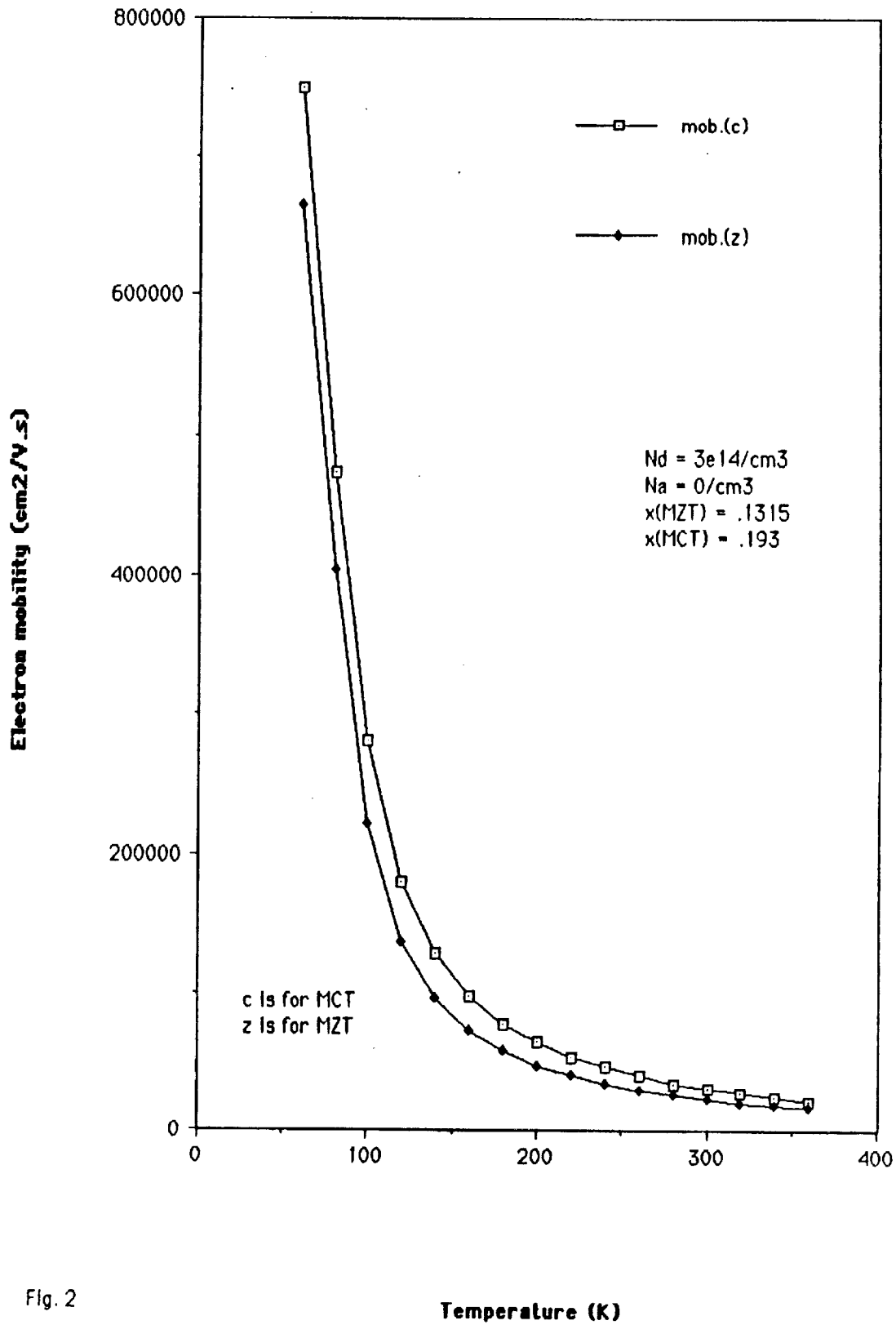


Fig. 2

Captions

Fig.1a MCT and MZT energy gap. $x(\text{MCT})=.193$, $x(\text{MZT})=.1315$

Fig.1b MCT and MZT electron concentration for the same energy gap.
 $N_d=3E14/\text{cm}^3$, $N_a=0/\text{cm}^3$, $x(\text{MCT})=.193$, $x(\text{MZT})=.1315$

Fig.1c MCT and MZT light hole concentration for the same energy gap.
 $N_d=3E14/\text{cm}^3$, $N_a=0/\text{cm}^3$, $x(\text{MCT})=.193$, $x(\text{MZT})=.1315$

Fig.1d MCT and MZT heavy hole concentration for the same energy gap.
 $N_d=3E14/\text{cm}^3$, $N_a=0/\text{cm}^3$, $x(\text{MCT})=.193$, $x(\text{MZT})=.1315$

Fig.2 MCT and MZT electron mobility for the same energy gap.
 $N_d=3E14/\text{cm}^3$, $N_a=0/\text{cm}^3$, $x(\text{MCT})=.193$, $x(\text{MZT})=.1315$

B. ABSTRACT FROM "ELECTRON MOBILITY IN n-TYPE $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ and $\text{Hg}_{1-x}\text{Zn}_x\text{Te}$ ALLOYS"

We have calculated the mobility of electrons in n-type Mercury Cadmium Telluride (MCT) and compared it to 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. Our major result is that for equivalent energy gaps, the mobilities in the two compounds are nearly the same. Since MZT is harder and structurally more stable with respect to Hg retention than MCT, this is a significant result. This calculation also appears to be the first extensive calculation of the mobility of MZT. The calculations for both MCT and MZT are based on sets of material parameters whose origin is described. 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 must be solved by a variational principle. We also discuss directions for future work and mention, in particular, the problem of characterizing donors.

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C. INTRODUCTION TO "THE EFFECTS OF SCREENING ON THE SCATTERING OF ELECTRONS BY NEUTRAL DEFECTS"

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We calculate the scattering of electrons by neutral defects in semiconductors both in the screened and the unscreened cases. If we have one kind of neutral defect whose number does not change with temperature (caused by vacancies, for example) and also neutral defects due to donors that have retained their electrons, then screening can have a significant effect for two reasons. One reason arises from the screening of the defect which increases with carrier concentration and hence with temperature. The other arises from certain special situations in which screening can cause an abrupt decrease in the number of neutral donors as the temperature is increased. Both of these effects will cause the importance of neutral defect scattering to increase as the temperature is lowered. We therefore argue that neutral defect scattering may be even more important at low temperature than one might expect.

The concept of screening of a charged impurity is well known, but the idea of screening a neutral impurity may seem strange. However as long as the potential due to the defect arises from an electrostatic potential it is susceptible to screening by conduction electrons. The charge distribution of the potential can be obtained from Poisson's equation. Neutrality would demand that the total charge be zero. For mathematical simplicity, we approximate this smoothly varying potential by a square well. Following the Brooks-Herring⁽¹⁾ treatment of ionized impurity scattering we calculate the inverse relaxation time in the Born approximation and treat the screening in the linearized approximation. We will comment on the approximations involved in this treatment below.

In order to estimate the screening of donors we do a variational calculation to see how the binding energy varies with screening. Coupling this with simple expressions for the variation of the concentration of donor electrons with binding energy and temperature and the dependence of the screening on electron concentration and temperature, we find a self consistent expression for the electron concentration at each temperature.

The idea is that electrons cause screening which reduces the binding energy which can cause more electrons. This effect can cause an abrupt change in the electron concentration in a narrow range of temperature. We investigate for what values of parameters this can be an important effect and find that special circumstances are needed.

Neutral impurity scattering has been treated by Erginsoy⁽²⁾, Sclar⁽³⁾, McGill and Baron⁽⁴⁾, Blagosklonskaya et. al⁽⁵⁾, Mattis and Sinha⁽⁶⁾, and Kwong et. al⁽⁷⁾. Most of these authors treated the neutral impurity like a hydrogen atom, although Sclar considered a strong short range potential similar to our model. Most authors find corrections to Erginsoy's prediction of an energy independent relaxation time.

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D. ABSTRACT FOR REPORT "IMPROVEMENT OF PROGRAM TO CALCULATE ELECTRONIC PROPERTIES OF NARROW BAND GAP MATERIALS"

Mercury Cadmium Telluride ($\text{Hg}_{1-x}\text{Cd}_x\text{Te}$) is a narrow gap semiconductor which is used for making infrared detectors and is a candidate for improved crystal growth in microgravity. We used a program for calculating the electron mobility and other properties which was written by Dr. S.L. Lehoczky and rewritten in BASIC by Ernestine Cothran. We have rewritten the program in FORTRAN both for a VAX 11/780 and a SUN workstation. We have investigated the sensitivity of the results to changes in the coupling of the electrons to the longitudinal optic phonons, to values for the low and high frequency dielectric constants, to disorder energy and to the number of acceptors. We have looked for the latest values of the energy gap as a function of x , heavy hole mass, dielectric constants as a function of x , and the momentum matrix element. We have examined how the mobility changes with changes in these quantities. We have found material parameters for the more stable compound Mercury Zinc Telluride and calculated its mobility as a function of temperature. We find that its mobility is comparable to Mercury Cadmium Telluride for the same energy gap. We have also examined the effect of different models for the donors. In the appendix we give an extensive list of relevant references, particularly as they apply to the theory. We also include a tutorial discussion of electron screening. Suggestions for future work include investigating the character of donors in as grown crystals, revisiting the theory of electron-longitudinal phonon interactions as treated in the "two mode theory" for these pseudo-binary compounds, looking again at the nature of hole scattering, trying to improve the treatment of scattering particularly as to dynamic effects. e.g. antiscreening, evaluating the screening parameters by the second Born approximation and the Friedel sum rule (where non parabolic effects are explicitly taken into account), and finally beginning to look at all the myriad effects that are introduced by multilayers.

E. ABSTRACT FOR GRANT PROPOSAL "FURTHER IMPROVEMENT IN PROGRAM TO CALCULATE ELECTRONIC PROPERTIES OF NARROW BAND GAP MATERIALS"

We propose to further improve a state of the art computer program originally written by Dr. S.L. Lehoczky. Our principal objectives will be to: (a) assess the accuracy of the effective charge used in characterizing electron-longitudinal optic mode scattering and improve as necessary, (b) review the characterization of donors and acceptors and thus try to improve ionized impurity scattering, (c) seek out all available mobility data, especially for Mercury Zinc Telluride, and compare it to our mobility calculations, (d) further improve our work on the table of parameters characterizing MZT and expand the work to other relevant crystals. Other work to be considered is given in the statement of work to be done (section IIC). The overall objective is to have a comprehensive program for calculating, as a function of temperature, mobility and related properties of a significant class of semiconductors. The program is to be accurate, flexible, and involve up to date data for input parameters.

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F. OUTLINE FOR TALK ON ELECTRON MOBILITY IN NARROW GAP
SEMICONDUCTOR

INTRODUCTION

Experiment vs Theory
Importance - Infrared
Radiation and Detectors
Applications

NARROW GAP SEMICONDUCTORS

MCT and complications

ELECTRON MOBILITY

Simple Model

INTERACTIONS

Screening - other
considerations

BOLTZMANN EQUATION

Variational Principle