Indirect Transitions in Indium Antimonide*

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An interpretation of published infrared absorption data for InSb is made. It is proposed that the absorption beyond the main optical edge is due to indirect transitions involving both optical mode and low-energy acoustical mode phonons.

RECENTLY a group at the Chicago Midway Laboratories (referred to hereafter as CML)[1] published some data (due to A. Goldberg and G. G. MacFarlane[1]) on the infrared absorption in a thick sample of indium antimonide. As can be seen from Fig. 1, a long-wavelength tail is evident. Roberts and Quarrington[2] also report a long-wavelength tail beyond the main absorption edge. MacFarlane and Roberts[3] explained these tails in Ge and Si as indirect optical transitions, utilizing phonons to conserve energy and to satisfy the selection rule $\mathbf{k}_i=\mathbf{k}_f+\mathbf{q}(k\theta)$, where $\mathbf{k}_i$ and $\mathbf{k}_f$ refer to the initial and final wave vector of the electron and $\mathbf{q}(k\theta)$ refers to the wave vector of the phonons involved. Empirically MacFarlane and Roberts and CML fit their data to an equation of the form

$$K=A^2\left\{\frac{[\hbar\omega-(E-k\theta)]^2}{e^{\theta/T}-1}+\frac{e^{\theta/T}}{e^{\theta/T}-1}[\hbar\omega-(E+k\theta)]^2\right\}.$$

The first term in the brace represents the absorption of a photon of energy $\hbar\omega$ and of a phonon of energy $k\theta$, the second term the absorption of a photon and the emission of a phonon. Bardeen, Blatt, and Hall[4] have given some theoretical justification for this square power law for optical absorption due to indirect processes.

CML fitted its data with two acoustical-mode phonons of $\theta=100°$K and $\theta=30°$K. It is the purpose of this note to suggest that an equally good fit to the data can be made by using four phonons. These comprise the two optical modes of $\theta=250°$K and $\theta=290°$K, and two low-energy acoustical modes which can be approximated by a single distribution of 8°K phonons [$A=111$ (cm$^{\frac{1}{2}}$ ev)$^{-1}$ in all cases]. Figure 1 shows the individual values of $K^{\frac{1}{2}}$ and the total $K^{\frac{1}{2}}$ for comparison with CML data. If we consider that the electron can interact with the longitudinal modes only, a similar fit can be made by adjusting the value for A. In either case, the absorption curve may be fitted with a combination of the higher energy optical modes and very low energy acoustical modes.

Figure 2(a) shows the spectrum of phonons for a small part of the reduced zone. The value of $\hbar\omega/k=250°$K is based on the reststrahlen frequency determined by Spitzer and Fan[5] and Yoshinaga.[6] That InSb

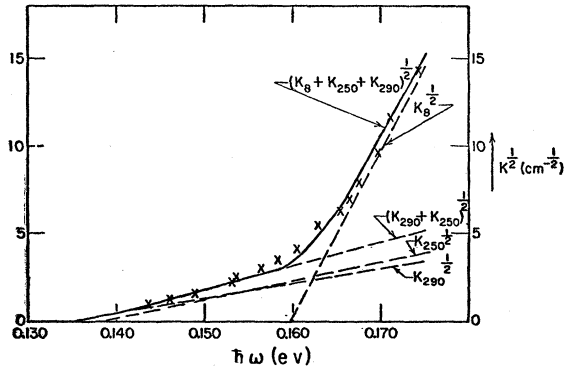

FIG. 1. The absorption edge of InSb. The × symbols indicate the experimental data of CML. The K_{290} and K_{250} curves were calculated by considering phonon absorption only.

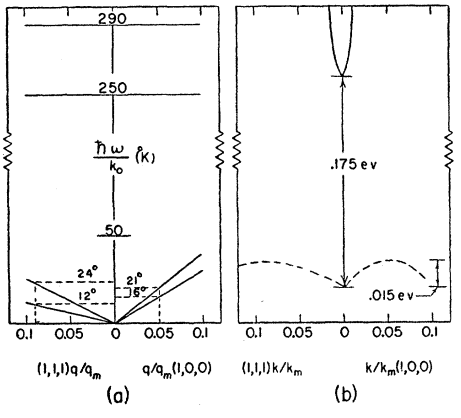

FIG. 2. (a) Vibrational spectra of InSb for the (1,0,0) and (1,1,1) axes. (b) Two possible electronic energy band profiles for InSb [$q_m(1,0,0)=k_m(1,0,0)=2(\pi/a_0)$ and $q_m(1,1,1)=k_m(1,1,1)=\sqrt{3}(\pi/a_0)$, where a_0 is the lattice constant].

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[1] Blount, Callaway, Cohen, Dumke, and Phillips, Phys. Rev. **101**, 563 (1956).

[2] V. Roberts and J. E. Quarrington, J. Electronics **1**, 152 (1955).

[3] G. G. MacFarlane and V. Roberts, Phys. Rev. **97**, 1714 (1955); **98**, 1865 (1955).

[4] Bardeen, Blatt, and Hall, in *Proceedings of the Atlantic City Photoconductivity Conference 1954* (John Wiley and Sons, Inc., New York, 1955). H. Brooks, in *Advances in Electronics and Electron Physics VII* (Academic Press Inc., New York, 1955) p. 166. A thorough but concise discussion of direct and indirect transitions can be found in the latter reference.

[5] W. G. Spitzer and H. Y. Fan, Phys. Rev. **99**, 1893 (1955).

[6] H. Yoshinaga, Phys. Rev. **100**, 753 (1955).

is slightly ionic is discussed in reference 5; thus the degeneracy of the optical modes is partly removed. We estimated the longitudinal optical mode to be 290°K by using an expression due to Mott and Fröhlich.[7] It has been assumed that the optical modes do not change with q over the small portion of the zone shown. It is the low-energy acoustical phonons which determine the value of $q(k\theta)$ to be used in the optical selection rule. The acoustical spectrum was determined from elastic constants of InSb.[8]

In Fig. 2(b) are shown two possible valence band structures, one with the maximum along the (1,0,0) axis assuming 21° and 16° phonons giving $q(k\theta)=0.05q_m$, the other with its maximum along the (1,1,1) axis assuming 24° and 12° phonons giving $q(k\theta)=0.09q_m$. It is assumed that the minimum of the conduction band is at the center of the zone (0,0,0), i.e., $\mathbf{k}_f=0$; thus $\mathbf{k}_i=\mathbf{q}(k\theta)$. As discussed in CML and by Parmenter[9] and Dresselhaus,[10] other alternatives are permitted by symmetry considerations.

The valence band energy profiles are shown as parabolas. If this is a valid assumption, and the maximum lies on the (1,1,1) axis, the effective mass for holes is $1.35m_e$. This is not inconsistent with the value $m^*>1.2m_e$ determined from the cyclotron resonance experiment.[11]

This suggested band structure is also consistent with two other experimental facts. Fan and Gobeli[12] recently reaffirmed in a thin sample of InSb that the optical gap is 0.175 ev. The thermal gap at 300°K is 0.160 ev as determined by Breckenridge *et al.*[13]

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[8] R. F. Potter, Bull. Am. Phys. Soc. Ser. II, **1**, 53 (1956).
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Vacancies and Displacements in a Solid Resulting from Heavy Corpuscular Radiation

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The number of displacements $D(E)$ and the number of vacancies $V(E)$ produced in a monatomic solid as a result of collisions due to an incident ion of initial energy E, are obtained as solutions of the equation

$$f(E)=\int_0^E dyK(E,y)\{p(y)[f(y-\alpha)+1-\theta q(E-y)]+[1-p(E-y)q(y)]f(y)\},$$

where $f(E)=D(E)$ or $V(E)$, $p(y)$ denotes the probability that a struck atom is displaced when it has received energy y, $q(E-y)$ is the probability that the striking atom replaces it if displacement has occurred, $K(E,y)$ is the scattering kernel, and α is the minimum amount of energy that is assumed to be necessary to displace an atom (it is assumed that the struck atom loses energy α in breaking away from its lattice site). In the equation, $f(E)=0$ for $E<\alpha$, with $\theta=0$ for displacements and $\theta=1$ for vacancies.

This equation is solved for some representative cases of $p(y)$ and $q(y)$. The functions $p(y)$ and $q(y)$ can be chosen to fit experimental estimates of either $D(E)$ or $V(E)$ singly but indicate a fundamental discrepancy of the joint estimates. The discrepancy, if not due to inaccuracy in the interpretation of experimental results, suggests that a mathematical model based on individual collisions is inadequate.

I. INTRODUCTION

IN previous investigations[1,2] the authors have determined the number of displacements $D(E)$ and the number of vacancies $V(E)$ in a monatomic solid produced as a result of collisions due to an incident atom of initial energy E. These calculations were based on a simple mathematical model characterized by a displacement energy α of the lattice atoms and the energy distribution of the struck atoms was determined by using the cross sections for collisions with free atoms. Taking y as the energy of the struck atom after the collision, we made the following assumptions:

(A) A displacement is produced whenever $y>\alpha$.

(B) A replacement is produced whenever $y>\alpha$ and $E-y<\alpha$.

Thus, a vacancy is produced whenever $y>\alpha$ and $E-y>\alpha$. The displacement energy α is often taken as about 25 ev.

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[2] J. Neufeld and W. S. Snyder, Phys. Rev. **99**, 1326 (1955).