Optical Absorption Edge of Compensated Germanium

Frank Stern
IBM Watson Research Center, Yorktown Heights, New York 10598
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The optical absorption of heavily doped and closely compensated Ge is calculated using a Halperin-Lax band-tail model and an *ad hoc* matrix element. The only adjustable parameter is an effective temperature T_{ion} for the contribution of the position correlations of the ions to the screening; T_{ion} is estimated to be about 7000 °K. The results are in reasonable agreement with experiment; direct transitions at $k=0$ make the dominant contribution to the edge.

A striking example of an absorption-edge tail in a semiconductor is the one found by Fowler, Howard, and Brock[1] in a closely compensated sample of Ge which had about 10^{20} donor atoms/cm^3 and an approximately equal number of acceptor atoms, with as few as 2×10^{17} electrons/cm^3 in some regions. Their absorption edge is about 0.1 eV lower in energy than the edge in pure Ge. We have used the density-of-states model of Halperin and Lax,[2] and an *ad hoc* matrix element described elsewhere,[3] to calculate the optical absorption for this material.

The screening length L_{scr}, which characterizes the coherence of the potential fluctuations, is a major parameter in these calculations. If the total concentration of donors and acceptors is held constant and the degree of compensation is increased, then the screening length increases and the potential fluctuations become large. If only free carriers contribute to the screening, then the fluctuations become unphysically large. Many authors[4-6] have proposed that the ions themselves participate in the screening, because they are mobile at the elevated temperatures at which the lattice is usually formed.

We approximate the screening length by the expression

$$L_{scr}=\left[\frac{4\pi e^2}{\kappa}\left(\frac{n}{E_{d,e}}+\frac{p}{E_{d,h}}+\frac{N_D+N_A}{KT_{ion}}\right)\right]^{-1/2}, \quad (1)$$

where $E_{d,e}$ and $E_{d,h}$ are the energies which enter into the Einstein relation[7] for electrons and holes (they equal KT for nondegenerate statistics), n and p are the electron and hole concentrations, N_D and N_A are the donor and acceptor concentrations, κ is the dielectric constant, K is Boltzmann's constant, and T_{ion} is an effective temperature for ion screening. We treat T_{ion} as an adjustable parameter.

Figure 1 shows the calculated optical absorption for $T_{ion}=7000$ and 9000 °K, together with the experimental results for compensated Ge [1] and for pure Ge,[8] all at 300 °K. Most of the details of the calculation are the same as those described elsewhere.[3] In particular, we have included an empirical carrier-induced band-gap shrinkage proportional to $n^{1/3}$, whose value for the case considered here is 15.7 meV. For the indirect transitions, we used the same energy-independent phonon-induced matrix element as the one deduced from the absorption in pure Ge. The effect of localization on the indirect transition is negligible in our model. On the other hand, the experiments in impure Ge suggest that this matrix element increases in doped samples,[9] an effect which may be due to mixing of the $k=0$ wave functions with those of the conduction-band minimum at L because of the presence of the impurities.

An enhanced matrix element for indirect transi-

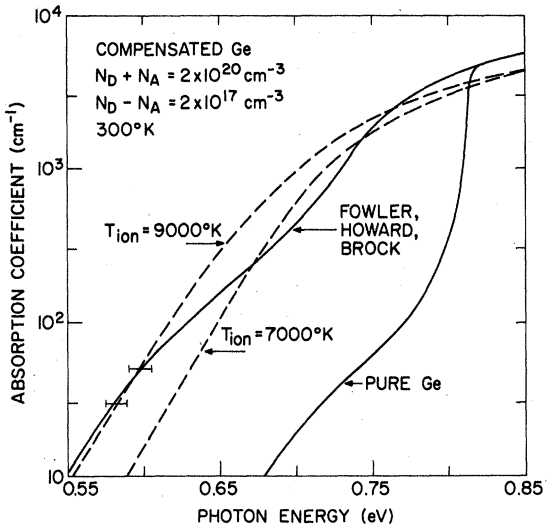

FIG. 1. Optical absorption of compensated Ge at 300 °K. The two dashed curves are calculated with effective temperatures for ion screening equal to 9000 and 7000 °K. The solid curves give the experimental results of Fowler, Howard, and Brock (Ref. 1), and, for comparison, the results for pure Ge of Dash and Newman (Ref. 8). Free-carrier absorption has been subtracted. The horizontal bars indicate the spread of experimental values from different measurements for low absorption coefficients, where the spread is greatest.

tions would improve the agreement between calculated and measured absorptions at low absorption coefficients (where the measured results are least reliable) in Fig. 1, but it is clear that even without this effect we can explain most of the shift of the absorption edge to lower energy using our band-tail model with the assumption that the effective temperature T_{ion} for screening of the ions by each other is about 7000 °K.

One might expect that a natural value for T_{ion} is the melting point, which is 1232 °K for Ge. But the Coulomb forces between the ions will be screened by the free carriers at elevated temperatures,[6] thus reducing the interaction. T_{ion} must be considered as a parameter which characterizes the ionic contribution to the screening via Eq. (1), rather than as a physical temperature. Our estimated value of 7000 °K corresponds to considerably less screening, and therefore to more band tailing, than would obtain with a value of T_{ion} near the melting point. The simple screening model that leads to (1) is a crude approximation, because the ions are rigid and produce an irregular screening pattern, unlike the smooth screening effect due to the average motion of the free carriers. (The free carriers present at a given temperature will tend to smooth out the irregularities due to the ions.) It is unlikely that a single screening length (1) can adequately represent the radial correlations between the ions.[10] Equation (1) does, however, provide a simple way to account for screening by the ions.

Our model gives reasonable agreement with experiment, and supports the conjecture[1] that direct transitions dominate the absorption edge in closely compensated Ge.[11]

I have enjoyed useful conversations with D. L. Mitchell and T. N. Morgan about the theory and with A. B. Fowler and W. E. Howard about their experimental results, and thank S. M. Hu for calling a reference to my attention.

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[1]A. B. Fowler, W. E. Howard, and G. E. Brock, Phys. Rev. 128, 1664 (1962). I am indebted to W. E. Howard for making the original data plots available.

[2]B. I. Halperin and M. Lax, Phys. Rev. 148, 722 (1966).

[3]Preliminary results for our model have been presented earlier: F. Stern, Bull. Am. Phys. Soc. 14, 396 (1969); J. Non-Cryst. Solids 4, 256 (1960); a manuscript describing its application to GaAs is in preparation; paper on the application of these ideas to amorphous Si is published in Phys. Rev. B 3, 2636 (1971).

[4]E. O. Kane, Phys. Rev. 131, 79 (1963), see discussion after Eq. (10).

[5]L. V. Keldysh and G. P. Proshko, Fiz. Tverd. Tela 5, 3378 (1963) [Sov. Phys. Solid State 5, 2481 (1964)], Eq. (8).

[6]M. I. Dyakonov, A. L. Efros, and D. L. Mitchell, Phys. Rev. 180, 813 (1969).

[7]See, for example, F. Stern, Phys. Rev. 148, 186 (1966).

[8]W. C. Dash and R. Newman, Phys. Rev. 99, 1151 (1955).

[9]C. Haas, Phys. Rev. 125, 1965 (1962); J. I. Pankove, in *Progress in Semiconductors*, edited by A. F. Gibson and R. E. Burgess (Heywood and Co., London, 1965), Vol. 9, p. 63.

[10]B. A. Volkov and V. V. Matveev, Fiz. Tverd. Tela 8, 717 (1966) [Sov. Phys. Solid State 8, 574 (1966)]; N. A. Brynskikh and A. A. Grinberg, Fiz. Tekh. Poluprov. 4, 1015 (1970) [Sov. Phys. Semiconductors 4, 869 (1970)].

[11]The relative contribution of the direct and indirect gaps can be tested by studying the effect of pressure and strain on the absorption edge. However, these measurements probably require larger and more homogeneous samples than those used in the work of Ref. 1. I am indebted to M. I. Nathan for suggesting and exploring the possibility of such experiments.