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ELECTRONIC STATES ON DISLOCATIONS IN SEMICONDUCTORS*

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Shockley[1] has suggested that "dangling bonds" along dislocations having partially edge character may give rise to acceptor levels in valence semiconductors. Landauer[2] investigated the trapping effects due to the dilatation only about an edge dislocation in Ge and found that this part of the strain field gives rise to a state bound only by 3×10^{-3} ev. Since the many-valley nature of a semiconductor may be expected to give rise to strong coupling between the electrons and the shear part of the elastic field, it seems profitable to examine states associated with dislocations using a more complete picture of the strain field and band structure. We have considered the (pure shear) strain field of the screw dislocation which presumably has no dangling bonds and made a preliminary study of the fields associated with dislocations of edge and sixty-degree types in n-type Ge. In all cases the strain field is found to give rise to states about 0.05 ev below the conduction band edge.

Within the framework of effective-mass and deformation-potential theories the interaction between the ith conduction band valley and the elastic field may be written as[3]

$$\delta E^{(i)} = \Xi_d \Delta + \Xi_u \sum_{k,l} n_k^{(i)} n_l^{(i)} u_{kl}. \tag{1}$$

Here Ξ_d and Ξ_u are the deformation potential constants, Δ is the dilatation, $n_k^{(i)}$ are the direction cosines of the band minimum in k space, and u_{kl} are the strain field components. In Ge the conduction band valleys lie at the zone boundary in $\langle 111\rangle$ directions.

The screw dislocation axis and Burgers vector lie in a $\langle 110\rangle$ direction which is taken as the z axis. The coordinate system and relevant crystallographic information are given by Fig. 1. Taking the strain field given by continuum elasticity theory we find that only those valleys lying in the $(1\bar{1}0)$ plane are affected. To find the lowest state on the dislocation we neglect the z motion and obtain

$$H = -\frac{\hbar^2}{2m_t}\left(\frac{\partial^2}{\partial x^2} + \frac{1}{K}\frac{\partial^2}{\partial y^2}\right) - \frac{\sqrt{2}\, b\, \Xi_u}{6\pi}\left(\frac{\gamma x}{x^2+\gamma^2 y^2}\right), \tag{2}$$

as the Hamiltonian for the bound states. Here m_t is the transverse effective mass and b the Burgers vector. $K = 3m_t m_l(m_t + 2m_l)^{-1}$, where m_l is the longitudinal effective mass. The elastic anisotropy factor is $\gamma = [(c_{11} - c_{12})/2c_{44}]^{1/2}$, the c's being the usual elastic constants. The potential in Eq. (2) is appropriate to the [111] valley. It is

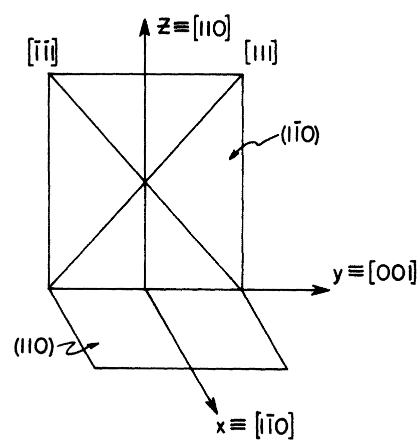

FIG. 1. Coordinate system used in treating the screw dislocation in Ge.

attractive for positive x and repulsive for negative x. The other valley in the $(1\bar{1}0)$ plane will have a sign change in the potential. Thus, we will have a twofold degeneracy, neglecting spin. One of these states will be localized on each side of the dislocation.

We choose a variational wave function of the form,

$$\psi=[(x^2+B^2y^2)^{1/2}+Ax]\exp[-C(x^2+B^2y^2)^{1/2}], \quad (3)$$

where A, B, and C are variational parameters. We use the values $b=4$ A, $\Xi_u=17$ ev.[3] Taking $m_t=0.0815\ m_e$ and $m_l=1.59\ m_e$ as given by Levinger and Frankl[4] (m_e = electronic mass), and $c_{11}=12.89$, $c_{12}=4.83$, $c_{44}=6.71$ (in 10^{11} dyne cm^{-2}) as given by Huntington,[5] we obtain a minimum variational energy of -0.045 ev (measured from the conduction band edge), corresponding to the values of the variational parameters $A=1.085$, $B=1.30$, $C=3.94\times10^6$ cm^{-1}. The wave function so obtained has a center of mass at $\langle x\rangle=35$ A from the dislocation and mean spreads of $[\langle x^2\rangle-\langle x\rangle^2]^{1/2}=27$ A and $\langle y^2\rangle^{1/2}=28$ A. These last values demonstrate the consistency of the use of effective-mass theory, and the position of the center of mass together with the spread shows that the bound state is not an artifact of the fictitious singularity of the continuum elasticity potential.

A lower limit for the ground state may be obtained by replacing the functional part of the potential in Eq. (2) by x^{-1} for $x>0$ and by 0 for $x<0$. This gives a potential which is everywhere lower than the correct one and whose ground state is therefore lower than the ground state of the system. The lowest state is then obtained in closed form and gives a lower limit of -0.08 ev.

Preliminary variational calculations have been made for the $\langle 112\rangle$ oriented edge and the $\langle 110\rangle$ sixty-degree dislocations neglecting elastic anisotropy. Again a bound state is found to lie about 0.05 ev below the conduction band edge. The very small binding energy predicted by Landauer is the result of neglecting the shear components of the strain field which are of dominant importance due to the many-valley nature of the conduction band and the relative magnitudes of Ξ_d and Ξ_u.

The experimental situation concerning the position in the gap of dislocation levels in Ge seems far from clear.[6] Different workers find themselves able to fit carrier depletion and recombination data using a wide variety of levels.[7] It has been suggested that some of the deep levels (if any) associated with dislocations are the consequence of impurity effects.[6] The levels predicted in the present note lie significantly deeper than common donor levels and may be expected to be populated at least at low temperatures. Measurement of the carrier depletion due to screw dislocations at low temperature and associated optical experiments would seem to be crucial tests.

Recent optical measurements of the fine structure of the fundamental absorption edge in the silver halides have shown that the valence bands of these materials are "many-hilled" while the conduction band is centered at the center of the zone.[8] Thus, the shallow trapping of the holes observed in these materials may be due to interactions with dislocation shear fields via the mechanism considered here.

The present treatment considers a single electron trapped in the strain field of a dislocation. At equilibrium in n-type material there will be a certain low density of electrons on the line. The strong correlation produced by the Coulomb interaction in one dimension may be expected to "quench" the z motion (perhaps forming a "lattice" of electrons at very low temperature) and to account for the lack of observable "extra" conductivity along dislocation lines.

In conclusion, it appears that the strain fields associated with dislocations in semiconductors can give rise to acceptor levels near the top of the gap and that these may have a significant influence on the electronic properties of n-type material.

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