

Localized and delocalized states on intersecting dislocations

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The influence of the crossing of dislocations on the localization of electronic dislocation states is investigated. The dislocation structure is approximated by a graph without cycles. Expressions are obtained for the mobility threshold and for the condition under which delocalized dislocation states exist.

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1. INTRODUCTION

Experimental results¹⁻⁴ show that dislocations have a strong influence on the static and microwave conductivities of plastically deformed semiconductors. In a preceding paper⁵ these results were interpreted within the framework of a simple model. The dislocation system was regarded as a network whose links are one-dimensional disordered systems. If the dislocation density is low enough then, when the dislocation structure is disordered, the concentration of the network nodes is small and the localization length is $l \ll N^{-1/3}$. In this case it was possible to consider each link separately, and the system conductivity could be calculated as the conductivity of a network made up of macroscopic resistors of random value (since the lengths of the link were random). It was found that the microwave conductivity is independent of N , and the static conductivity is proportional to $\exp(-\text{const}/N^{1/3})$ and increases rapidly with increasing N .

When the dislocation density is increased, the concentration of the nodes increases the condition that the links are independent is violated at $l \sim N^{-1/3}$, since the boundary conditions for the wave functions at the nodes become of importance. The dislocation system can in this case not be regarded as a network of macroscopic resistors, and it is necessary to solve the Schrödinger equation for the entire dislocation system as a whole. The principal scattering mechanism in this case is not scattering by a random potential, but scattering by the nodes of the dislocation network. For this reason it is meaningful to neglect the scattering by a random potential and to consider only scattering by the nodes. Since the dislocation system is, generally speaking, random we have a specific disordered system: the motion over the links will be regarded as free, the links have random lengths, and are randomly interconnected. In addition, broken bonds located at the nodes differ from the bonds inside the links because of the rearrangements of the crystal structure.

When the system is disordered, the presence of connectivity of the dislocation network is not a sufficient condition for the existence of static conductivity, since the electronic states can be localized. The purpose of the present paper is to investigate the possible existence of localized and delocalized states in random dislocation networks of the described type, and by the

same token draw a definite conclusion concerning the static conduction over the dislocations.

2. THE MODEL

We replace the real dislocation system by the idealized one shown in Fig. 1. The broken bonds of the individual dislocations are marked by light circles and Greek letters. They correspond to wave functions φ_α and to energies ε_α . The broken bonds corresponding to the nodes are designated by dark circles and Latin letters. The node bonds corresponded to φ_i and ε'_i . The overlap integrals $V = \int \varphi_\alpha^* H \varphi_\beta dr$ differ from zero only for the nearest neighbors and are constant for all bonds. Thus, the perturbation introduced by the nodes has an extremely short range of action.

The number of dislocations that converge at a node i will be designated ω_i . We consider only structures for which $\omega_i = \omega$ is constant. The length R_{ij} of the links or the number of atoms N_{ij} in a link is constant. For simplicity we assume that the different R_{ij} are statistically independent and that the probability density of an individual link is given by

$$\varphi(R) = \begin{cases} \Delta^{-1}, & |R - R_0| < \Delta/2 \\ 0, & |R - R_0| > \Delta/2, \end{cases} \quad (1)$$

with $R_0 > \Delta/2 \gg a$, where a is the distance between the broken bonds.

A real dislocation structure is also characterized by the fact that individual links are interconnected randomly (with account of the assumed condition $\omega_i = \omega$). The resultant networks can be topologically most varied. Experimental investigations allow us to state that all have one common property, namely, they do not contain any closed cycles with small numbers of steps. From among those observed in experiment, the smallest number steps n in a cycle is possessed apparently by a hexagonal network of dislocations ($n = 6$). Using the condition $n \gg 1$, would replace a real

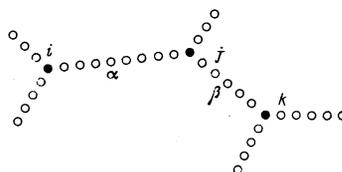


FIG. 1.

dislocation network by a graph without cycles, i. e., by a tree.

3. BASIC EQUATIONS

Each broken bond is characterized either by a number α_{ij} (if one counts from the point i to the point j), or by a number α_{ji} (counting from j to i). It is convenient to consider each link twice, both ij and ji , so as to avoid the problem of determining the start and the end of the link. We seek the solution of the Schrödinger equation in the form

$$\psi(\mathbf{r}) = \frac{1}{2} \sum_{ij} \sum_{\alpha_{ij}}' a^{ij}(\alpha_{ij}) \varphi^{ij}(\mathbf{r}, \alpha_{ij}). \quad (2)$$

The factor $1/2$ in front of the sum is due to the fact that each link is counted twice, as ij and as ji . For the same reason, the terms $\alpha_{ij}=1$ must be divided by ω , a fact designated by the prime of the inner summation sign.

At $\alpha_{ij} \neq 1$, N_{ij} , we have for $a^{ij}(\alpha_{ij})$ the equations

$$(\epsilon_0 - \epsilon) a^{ij}(\alpha_{ij}) + V (a^{ij}(\alpha_{ij} + 1) + a^{ij}(\alpha_{ij} - 1)) = 0. \quad (3)$$

They are satisfied if

$$a^{ij}(\alpha_{ij}) = A^{ij} \exp \{ika(\alpha_{ij} - 1)\} + B^{ij} \exp \{-ika(\alpha_{ij} - 1)\}, \quad (4)$$

$$\epsilon = \epsilon_0 + 2V \cos ka. \quad (5)$$

The variables A^{ij} and B^{ij} are determined by the equations for the node links and by the symmetry conditions. The former take the form

$$(\epsilon_0' - \epsilon) a_i^{ij} + V \sum_j a_j^{ij} = 0, \quad (6)$$

where the sum is over ω nearest neighbors. The latter can be written in the form

$$a_i^{ij} = M^i, \quad j = 1 \dots \omega, \quad (7)$$

$$a^{ij}(\alpha_{ij}) = a^{ji}(N_{ij} + 1 - \alpha_{ij}). \quad (8)$$

Equation (7) is obtained if it is recognized that a_i^{ij} pertains to one and the same node bond regardless of the value of j . In exactly the same manner, Eq. (8) means that $a^{ij}(\alpha_{ij})$ and $a^{ji}(N_{ij} + 1 - \alpha_{ij})$ pertain to one of the same bond inside the link. Substituting in Eq. (4) in Eqs. (6)–(8), we obtain a system of equations for A^{ij} and B^{ij} .

Investigation of this system can yield

$$A^{ij} = (B^{ij})^*.$$

Next, introducing the variables $\text{Re}A^{ij}$, $\text{Im}A^{ij}$, and then eliminating $\text{Im}A^{ij}$, we obtain a system for $\text{Re}A^{ij} \equiv m_i$:

$$(\epsilon_i - \epsilon) m_i + \sum_j v_{ij} m_j = 0; \quad (9)$$

$$\epsilon_i = \epsilon_0' + V \omega \cos ka - V \sin ka \sum_j \text{ctg} kR_{ij}, \quad (10)$$

$$v_{ij} = V \sin ka / \sin kR_{ij}.$$

In the sum j denotes the nearest neighbors of i .

The condition for the existence of a nonzero solution (9) with account taken of Eqs. (5) and (10) yields a very complicated transcendental equation for k . The complex solutions of this equation correspond to defect states localized near the nodes. The energies of these states lie outside the band $(\epsilon_0 - V, \epsilon_0 + V)$. These

states are similar to the usual surface states of a finite crystal. Real solutions correspond to states delocalized over the link. Their energies lie in the band $(\epsilon_0 - V, \epsilon_0 + V)$.

Delocalization along the link still does not mean delocalization in the entire dislocation system. To determine which of the states of the band $\epsilon = \epsilon_0 + 2V \cos ka$ are localized and which are delocalized, we turn to the system (9). It can be regarded formally as a Schrödinger equation in the strong-coupling approximation for a disordered system with random node energies ϵ_i and with random overlap integrals v_{ij} .

By determining the energy ϵ_c that separates the localized and delocalized states in such a disordered system, we can draw certain conclusions for the initial problem of localization on a dislocation network.

4. DETERMINATION OF THE LOCALIZATION THRESHOLD

A self-consistent method of describing localization, which yields an exact solution in the case of networks without closed cycles, was developed in Ref. 6. The system investigated there is described by Eqs. (9) with $v_{ij} = \text{const}$ and with random ϵ_i . A generalization to the case of both v_{ij} and ϵ_i random (even for dependent v_{ij} and ϵ_i) consists of changing the concrete formulas. The general idea, however, remains the same. We therefore describe the solution very briefly, referring the reader to Ref. 6 for detail. We introduce first the notation and determine the statistical properties of ϵ_i and v_{ij} . Assume that we are considering two nodes i and j . It is convenient to express ϵ_i in the form

$$\epsilon_i = A + B \sum_{l=\infty}^{\infty} \zeta_{il} + B \zeta_{ij} = \eta_i + B \zeta_{ij}; \quad (11)$$

$$\zeta_{ij} = \text{ctg} kR_{ij}, \quad A = \epsilon_0 + V \omega \cos ka, \quad B = -V \sin ka.$$

Accordingly

$$v_{ij} = -B(1 + \zeta_{ij}^2)^{1/2}. \quad (12)$$

The quantity η_i is statistically independent of ζ_{ij} , and consequently of v_{ij} . Taking into account Eq. (1) we obtain for the probability density η the expression

$$p(\eta) = \frac{1}{\pi} \frac{(\omega - 1) |B|}{(\eta - A)^2 + (\omega - 1)^2 B^2} \quad (13)$$

and correspondingly for ζ :

$$q(\zeta) = \frac{1}{\pi} \frac{1}{1 + \zeta^2}. \quad (14)$$

Since the lengths of the individual links are statistically independent, η and ζ are also independent.

Following Ref. 6, we write down equations for the real and imaginary parts of the self energy $S_i(\epsilon) = E_i + i\Delta_i$, which in our case take the form (ϵ is the energy)

$$E_i = \sum_j' \frac{B^2(1 + \zeta_{ij}^2)(R - \eta_j - E_j - B\zeta_{ij})}{(R - \eta_j - E_j - B\zeta_{ij})^2 + (\delta + \Delta_j)^2}, \quad (15)$$

$$\Delta_i = \sum_j' \frac{B^2(1 + \zeta_{ij}^2)(\delta + \Delta_j)}{(R - \eta_j - E_j - B\zeta_{ij})^2 + (\delta + \Delta_j)^2}, \quad (16)$$

where the summation is over $\omega - 1$ neighbors, $R = \text{Re} \epsilon$,

and $\delta = \text{Im}\epsilon \rightarrow 0$. Equations (15) and (16) are exact only for networks without cycles.

We investigate next the probability density of the quantities E_j and Δ_j , which we designate $f(E_j, \Delta_j)$. Using (13)–(16), we can calculate $f(E_i, \Delta_i)$ and, identifying it with $f(E_j, \Delta_j)$, obtain an integral equation for f . It is convenient to write it in the form of an equation for the Fourier transform f of the function $F(k_1, k_2)$:

$$F(k_1, k_2) = \left\{ \frac{1}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dx d\zeta dk_1' q(\zeta) P(k_1') F \left[k_1', k_2 B^2 \frac{(1+\zeta^2)}{x^2} \right] \right. \\ \left. \times \exp \left[ik_1' (R - B\zeta) - ik_2 \frac{B^2(1+\zeta^2)}{x^2} \delta - ik_1' x - ik_1 \frac{B^2(1+\zeta^2)}{x} \right] \right\}^{\omega-1}. \quad (17)$$

Here $P(k_1')$ is the Fourier transform of the function $p(\eta)$. We used also the fact that for localized states [it is precisely for them that Eq. (17) is satisfied] we have $\delta \rightarrow 0$ as $\Delta \rightarrow 0$.

Corresponding to localized states are also those solutions of (17) which yield, with unity probability, $\Delta \rightarrow 0$ as $\delta \rightarrow 0$. It is possible to determine the condition for the existence of such solutions and by the same token to determine exactly the localization criterion by means of a numerical solution. It is much simpler to find an approximate localization criterion. Following Anderson,⁷ we put $E_i = 0$. Then, substituting $ik_2 \rightarrow s$, we obtain from (17)

$$F(s) = \left\{ \int_{-\infty}^{\infty} dx d\zeta q(\zeta) p(R - x - B\zeta) \right. \\ \left. \times F \left[\frac{sB^2(1+\zeta^2)}{x^2} \right] \exp \left[-\frac{sB^2(1+\zeta^2)\delta}{x^2} \right] \right\}^{\omega-1}. \quad (18)$$

The localization criterion can be obtained by investigating the behavior of $F(s)$ at small s . Putting $F(s) = 1 - As^\beta$ with $\beta \in (0, 1/2)$, we find from (18) (see Ref. 6)

$$(\omega-1)B^{2\beta} \int_{-\infty}^{\infty} dx d\zeta q(\zeta) p(R - x - B\zeta) \frac{(1+\zeta^2)^\beta}{x^{2\beta}} = 1. \quad (19)$$

Localized states exist so long as Eq. (19), as an equation for β , has solutions in the interval $(0, 1/2)$. Using (13) and (14) and calculating the integral with respect to dx , we can reduce Eq. (19) to the form

$$\frac{(\omega-1)^{\beta(1-\beta)}}{\pi \cos \pi\beta} \int_{-\pi/2}^{\pi/2} d\varphi \cos 2\beta\varphi \{ [(\omega-1) \sin \varphi - D \cos \varphi]^2 + \cos^2 \varphi \}^{\beta-1} = 1, \quad (20) \\ D = (R - \epsilon_0' - V \omega \cos ka) / V \sin ka.$$

Investigating (20) numerically, we obtain the condition for the existence of localized states

$$|D| > D_c(\omega).$$

The constants $D_c(\omega)$ are equal to 6.9, 10.6, and 14.1 respectively for $\omega = 3, 4$, and 5.

5. CONCLUSIONS

Using the results of the preceding sections, we can describe the general structure of the spectrum of the model under consideration. Figure 2 shows schematically the state density. As already noted in Sec. 3, there exist solutions with complex values of k and

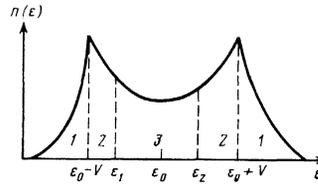


FIG. 2.

localized near nodes. Their energies lie outside the band $(\epsilon_0 - V, \epsilon_0 + V)$ and form regions marked 1 on Fig. 2. Inside the band $(\epsilon_0 - V, \epsilon_0 + V)$ there exist regions of localized (regions 2) and delocalized (region 3) states. The lower and upper localization thresholds $\epsilon_{1,2}$ are determined from Eqs. (5) and (21):

$$\epsilon_{1,2} = \epsilon_0 + \frac{(\epsilon_0 - \epsilon_0')(\omega-2) \mp VD_c [(\omega-2)^2 + D_c^2 - (\epsilon_0 - \epsilon_0')^2/V^2]^{1/2}}{(\omega-2)^2 + D_c^2}. \quad (22)$$

If

$$(\epsilon_0 - \epsilon_0')^2/V^2 \geq (\omega-2)^2 + D_c^2,$$

then all the states in the band are localized. For $\omega = 3$ this takes place at $|\epsilon_0 - \epsilon_0'| \geq 7V$. We note that the determined localization thresholds are approximate only because of the approximate solution of Eq. (17). The method itself makes it possible to obtain them exactly. To interpret the experimental data, however, there is no need for exact solutions, since the model itself contains definite approximations.

Comparing the results with the preceding paper⁵ we can draw the following conclusion. Crossings of dislocations, besides violating the one-dimensionality (the delocalization effect), introduce an additional scattering mechanism (localization effect). For the existence of static conduction over the dislocations it is necessary at the very least that the disorder introduced by the sections be weak, namely

$$(\epsilon_0 - \epsilon_0')^2/V^2 < (\omega-2)^2 + D_c^2(\omega). \quad (23)$$

We emphasize furthermore that the considered model is applicable to all (not necessarily dislocation) random networks made up of one-dimensional elements.

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¹Yu. A. Osip'yan and S. A. Shevchenko, Pis'ma Zh. Eksp. Teor. Fiz. 20, 709 (1974) [JETP Lett. 20, 328 (1974)].

²V. A. Grazhulis, V. Yu. Mukhina, Yu. A. Osipyan, and S. A. Shevchenko, Zh. Eksp. Teor. Fiz. 68, 2149 (1975) [Sov. Phys. JETP 41, 1076 (1975)].

³V. A. Grazhulis, V. V. Kveder, V. Yu. Mukhina, and Yu. A. Osip'yan, Pis'ma Zh. Eksp. Teor. Fiz. 24, 164 (1976) [JETP Lett. 24, 142 (1976)].

⁴Yu. A. Osip'yan, V. I. Tal'yanskiĭ, and S. A. Shevchenko, Zh. Eksp. Teor. Fiz. 72, 1543 (1977) [Sov. Phys. JETP 45, 810 (1977)].

⁵I. A. Ryzhkin, Fiz. Tverd. Tela (Leningrad) 20, 3612 (1978) [Sov. Phys. Solid State 20, 2087 (1978)].

⁶R. Abou-Chacra, P. W. Anderson, and D. J. Thouless, J. Phys. C: Sol. St. Phys. 6, 1734 (1973).

⁷P. W. Anderson, Phys. Rev. 109, 1492 (1958).

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