Possible localization of electrons at dislocations, disclinations, and grain boundaries in metals

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The electronic structure of defects of various types in hexagonal and square lattices has been studied numerically. It is found that this structure is governed primarily by the core of the defect, rather than by the long-range part of the deformation potential. The conditions for localization of electrons depend on the type of lattice, the nature of the decay of the transport integrals, and the "local" symmetry of the defect. A study of disclinations shows that a fivefold axis promotes localization, in contrast with a sevenfold axis.

Numerous results on the effect of plastic deformation on the electrical resistance of metals[1–3] and on the effect of superconducting transitions on mechanical properties[4] indicate that the interactions of electrons and dislocations are important. The microscopic mechanisms for these interactions (e.g., the relative importance of the deformation potential and dangling bonds in a core) are not yet clear. The interpretations of given experimental data by different investigators are often contradictory (compare the discussions in Refs. 2 and 3 of the scattering of electrons by dislocations in Al). One reason for this situation is that the scattering of an electron by, for example, an edge dislocation is an extremely nontrivial problem even in the continuum model (variables cannot be separated in the Schrödinger equation). As a result, the approaches which have been taken, beginning with the pioneering study by Lifshits and Pushkarov,[5] have been limited to nonrigorous estimates of the energies of highly excited states. In the present letter we analyze structural features of real crystals which are associated with the basic types of defects: edge dislocations, disclinations, and grain boundaries. To the best of our knowledge, there has been no previous study of the electronic structure of the defects of the two latter types.

An edge dislocation is set up by introducing an extra plane. In a 2D lattice, the extra plane is an extra row of atoms, which ends at the origin of coordinates. We consider cases in which a cross section perpendicular to the axis of a dislocation is a hexagonal or square lattice, whose sites are numbered by the vectors $\rho=(x, y)$. The electronic structure is calculated in the strong-coupling approximation for the 2D model; i.e., the Schrödinger equation

$$i\frac{\partial\psi}{\partial t}=\sum_{\rho'} T(\rho-\rho')\psi(\rho') \qquad (1)$$

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is solved with various functional dependences for the transport integrals $T(R)$ [for s-wave functions, with $T=T(|\mathbf{R}|)$, and also with allowance for the angular distributions for the t_{2g} and e_g functions].[6] The coordinates of the atoms in the distorted lattice are calculated in the Peierls–Nabarro model,[7] which makes it possible to avoid divergences of the continuum elastic theory. The radius of the dislocation core, r_0, is varied from $0.5a$ to $2a$; the variation causes no qualitative changes in the results. In all the figures below we use the value $r_0=a$, where a is the lattice constant. If we adopt the nearest-neighbor approximation for $T(\mathbf{R}, \mathbf{R}')$ in the direction along the dislocation axis, z, i.e.,

$$T_{\mathbf{RR}'}=\begin{cases} T(\boldsymbol{\rho}-\boldsymbol{\rho}'), & z=z', \\ T_0, & \boldsymbol{\rho}=\boldsymbol{\rho}', \quad z=z'\pm 1, \\ 0, & \text{otherwise}, \end{cases} \tag{2}$$

then the 2D model has a rigorous foundation in the sense that the onset of a localized level with an energy E_0 corresponds to a dislocation zone $E(k_z)=E_0+2T_0\cos k_z$ in the 3D case.

The Cauchy problem for Eq. (1) was solved by a very simple simplex method (the leap-frog method),[8] which rigorously ensures the unitarity of the evolution operator. This method also makes it possible to find an exact value of the spectral function for a system of linear differential equations in the limit of an infinite integration time, through an appropriate change in energy. The local density of states at the site, $\boldsymbol{\rho}_0$, is determined by a Fourier time (t) transform of $\psi(\boldsymbol{\rho}_0, t)$ with the choice of initial condition $\psi(\boldsymbol{\rho}, 0)=\delta_{\boldsymbol{\rho}\boldsymbol{\rho}_0}$. To study the localization in real space in the specification of the energy E, we calculate the square of the Fourier transform (in time) of $\psi(\boldsymbol{\rho}, t)$ with the initial condition $\psi(\boldsymbol{\rho}, 0)=\text{const}$ (a localization of an initially "smeared" electron). A test of the method for ideal 2D lattices showed that it is highly accurate, even reproducing details of the Van Hove singularities. In the calculations we used clusters of $N\leqslant 1000$ atoms; it was found that this approach leads to results which are independent of N. For an isolated dislocation we used "free" boundary conditions, while for dislocation dipoles we also used periodic boundary conditions.

The results of the calculations show that the parameters of the localized states are highly sensitive to the type of lattice and to the dependence of $T(\mathbf{R})$ on the modulus of the vector $\mathbf{R}$, while these parameters are less sensitive to the angles of the latter vector. Figure 1 shows results calculated on the local density of states at the dislocation axis, $N_0(E)$, for a hexagonal lattice (the positions of the localized levels were determined with the help of the localization criterion mentioned above). The replacement of the $T(\mathbf{R})\sim 1/R^5$ dependence, characteristic of the Wannier functions for d-wave states, by $\exp(-\alpha R)$ with $\alpha\sim a^{-1}$ leads to a weakening of the localization [a decrease in the weight of the corresponding peak in $N_0(E)$ and a greater smearing of $|\psi(\boldsymbol{\rho}, E_0)|^2$]. When we switch to a square lattice, using the same $T(\mathbf{R})$ dependence, the localization is suppressed to an even greater extent, although the fact that there are local levels was established in all the cases which we studied. Apparently one of the most important results is the assertion that the dislocation core, rather than the tails of the deformation potential, plays a governing role for the electronic structure. This

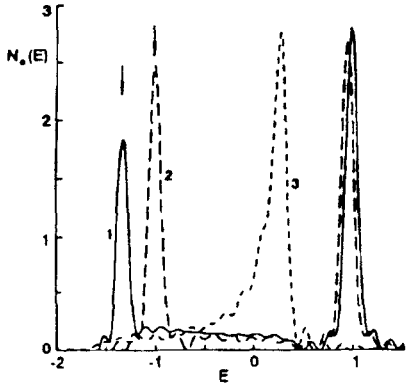

FIG. 1. Local densities of states $N_0(E)$ for a hexagonal lattice with $|T(\mathbf{R})| = 1/6R^5$ and with the angular distributions corresponding to an s–s bond (1) and a t_{2g} π bond (2). The arrows show the energies of localized states. 3—$|T(\mathbf{R})| = e^{-\alpha R}$, $\alpha = \ln(6)$, s–s bond. There is essentially no manifestation of localization here. The quantity R is expressed in units of the lattice constant a.

point is demonstrated by the essential agreement of the densities $N_0(E)$ for the cases of an isolated dislocation and of a dislocation dipole with an arm of $(2–3)a$.

Some other important structural elements of a real crystal are grain boundaries. We studied the electronic structure of a $\Sigma = 7$ tilt boundary on a hexagonal lattice with a rotation angle of 38.2° and with a $\langle 14\underline{5}0 \rangle$ normal to the plane of the boundary. The coordinates of the atoms were specified in a scheme of a lattice of coincident sites.[9] The results of these calculations (Fig. 2) show that the electronic structure of this boundary is surprisingly similar to that of a wall of edge dislocations, although the boundary discussed here cannot, in general, be regarded as a small-angle boundary. Along with the results calculated for dislocation dipoles, this result is evidence that the localiza-

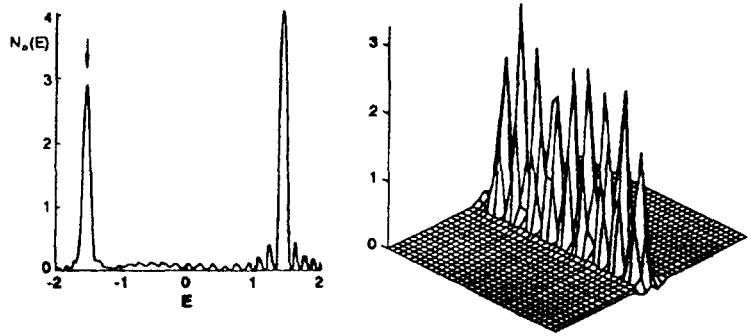

FIG. 2. Density of states $N_0(E)$ for a site at a tilt boundary (a) and distribution of the electron density at the energy of a localized state (b). Here $T(\mathbf{R}) = 1/(6R^5)$, where R is in units of the lattice constant a.

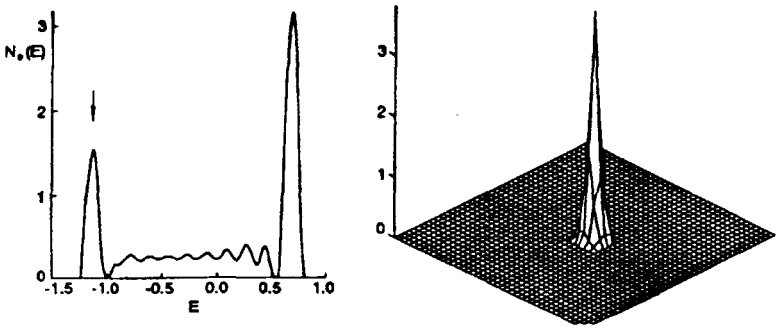

FIG. 3. Local density of states $N_0(E)$ (a) and distribution of the electron density at the energy of a localized state (b) for a pentagonal disclination. Here $T(\mathbf{R})=1/(6R^5)$, where R is again in units of the lattice constant a.

tion of electrons even in a very tight dislocation cluster occurs essentially at each dislocation separately (in the case at hand, we are talking about intrinsic grain-boundary dislocations).[9]

Yet another type of crystal defect which disrupts the rotational symmetry is a disclination. In addition to the "traditional" fields (e.g., descriptions of dislocation walls or a disclination dipole),[10] these defects have recently been attracting interest as structural elements of pentagonal particles.[11] They also arise in a natural way in a description of the structure of Frank–Kasper phases, quasicrystals, and glasses.[12] The electronic structure of a $+60°$ wedge disclination (pentagonal) and a $-60°$ disclination (heptagonal) was studied on a hexagonal lattice (the displacements of the atoms were specified on the basis of elastic theory).[10] In the latter case it was not possible to find localized states with any of the functional dependences $T(\mathbf{R})$ considered. Figure 3 shows the electronic structure of a pentagonal disclination. It is qualitatively like the electronic structure of an edge dislocation. The coordinations of the atoms in the core of these two defects are the same, while the deformation potentials are quite different at long range. On the other hand, the potentials differ only in sign in the $+60°$ and $-60°$ cases. Consequently, the conclusion that the core plays a governing role for the electronic structure remains in force in the case of disclinations. In addition, one gets the impression that the presence of a "local" fivefold symmetry axis, in contrast with a sevenfold one, promotes the appearance of localized states. The latter circumstance may be of interest for analyzing the electronic structures of quasicrystals and glasses.[12]

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