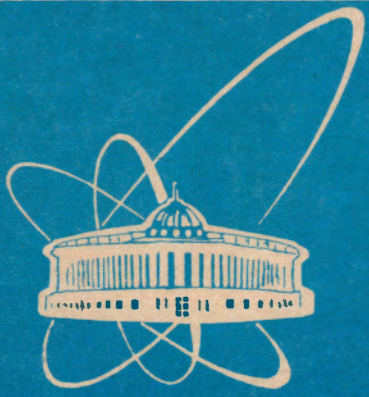

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LOCALISED ELECTRON STATES IN ELASTIC MATERIALS WITH DISCLINATIONS

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As is well known (see, e.g., [1]), the presence of defects even in minor concentrations can essentially modify electronic properties of materials, first of all semiconductors. This problem was studied in detail for point impurities [2] and linear translational defects - dislocations [3-6]. In both cases, the interaction of an electron with the longitudinal acoustic vibrations can result in localisation of the electron at defects. The electron states in disclinated materials are less well understood yet. Qualitative analysis performed recently in [7, 8] showed the possibility for the binding of electrons to negative disclinations.

In this Letter, we study the problem of an electron localisation in disclinated materials numerically in the context of the gauge model proposed in [9]. This model is the natural extension of the Edelen-Kadić gauge model [10] for elastic continuum with dislocations and disclinations. The interaction of electrons with elastic media is considered in the framework of the deformation-potential theory. The validity of the effective mass approximation is assumed. When the defect fields are considered as the external ones, the stationary Schrödinger equation takes the following general form (cf. [7]):

$$[-\sum_{A,B}\frac{\hbar^2}{2m^*_{AB}}D_AD_B+V(\vec{r})]\Psi_E(\vec{r})=E\Psi_E(\vec{r}). \qquad (1)$$

Here m^*_{AB} is the effective electronic mass tensor, and $V(\vec{r})$ is the deformation potential. The electron energy E is measured relative to the bottom of the conduction band in the undeformed crystal. As is seen, the most important deviation from the standard model is the replacement of the conventional derivative $\partial_A=\partial/\partial x_A$ by the covariant one D_A. In the presence of dislocations the translational symmetry of elastic media is broken, so that the gauge group is $T(3)$. In this case [11], the covariant derivative coincides with the conventional one, so that we arrive at the standard model known in dislocation theory [3-6].

For disclinations the gauge group is the rotational one. There are two kinds of symmetry which are appropriate for disclination problems. The first one is the spherical symmetry which occurs for point disclinations like the known 'hedgehog' in liquid crystals [12]. In this case the gauge group is $G=SO(3)$ and the covariant derivative is determined to be $(D_A\Psi)_j=\partial_A\Psi_j-i\varepsilon^\alpha_{jk}W^\alpha_A\Psi_k$ where W^α_A are the gauge fields due to disclinations and ε^α_{jk} is a completely antisymmetric tensor. The second kind of symmetry is the cylindrical one that holds for linear disclinations. In this case only rotations in the plane normal to the defect line are of importance, so that the gauge

group reduces to $G=SO(2)$. The covariant derivative takes then the form $D_A\Psi=(\partial_A-iW_A)\Psi$. Thus, for rotational defects a perturbation appears not only in the potential energy due to the deformation potential, but in the kinetic energy as well.

Let us restrict consideration to acoustic deformations. As is known [1], in general, there are six independent components of the deformation-potential tensor. For cubic crystals they can be reduced to two components, so that the deformation potential takes the form

$$V(\vec{r})=-G_dSpE_{AB}(\vec{r})-G_u\sum_{A,B}\eta_{AB}(\vec{r})(m^*_{AB})^{-1}D_AD_B \qquad (2)$$

where E_{AB} is the strain tensor and $\eta_{AB}=E_{AB}-\frac{1}{3}\delta_{AB}SpE_{AB}$. In the following, we will restrict consideration to materials of zinkblende or wurtzite structures where carriers belong to a singlet band centered at $\vec{k}=0$, $\vec{k}$ is the wave vector. The only strain component that can affect the energy of such a band is the dilatation, i.e. only the first term in (2) has to be taken into account. Accordingly, the effective mass tensor reduces to a scalar m^*.

Let us consider the linear disclination oriented along the z-axis. In this case, the exact solution of the problem was found to have a vortex-like form. Particularly, the gauge fields W_A were found to be [13]:

$$W_r=0,\quad W_\theta=W(r)=\nu/r,\quad W_z=0 \qquad (3)$$

where ν is the Frank index. The exact solution of the problem has been obtained for two cases: a) small ν, this corresponds to the partial topologically unstable disclinations, and b) $\nu=1$, a complete topologically stable disclination.

It is important to note that in either case the dilatation was found to depend only on the radial vector $\vec{r}$ in the xy plane. The electron wave function can be chosen as $\Psi_E(x,y,z)=\Psi_E(r,\phi)\Psi_E(z)$. Then, the stationary Schrödinger equation (1) is rewritten in the following form:

$$\Big(-\frac{1}{r}\frac{d}{dr}r\frac{d}{dr}+\frac{(j-\nu)^2}{r^2}-\frac{2m^*G_d}{\hbar^2}SpE_{AB}\Big)u^j_E(r)=k^2u^j_E(r). \qquad (4)$$

Here we have used the ansatz $\Psi_E(\vec{r})=\sum_j u^j_E(r)\frac{e^{ij\theta}}{\sqrt{2\pi}}$, $j=0,\pm1,\pm2,\ldots$; and $k^2=2m^*E/\hbar^2$. The effective potential in (4) consists of two parts, the deformation-potential energy and the so-called centrifugal energy, and takes the form

$$U_j(r)=-G_dSpE_{AB}+\frac{\hbar^2(j-\nu)^2}{2m^*r^2}. \qquad (5)$$

Let us note once more that the most important distinction from the case of dislocations and point impurities is that the interaction of an electron with the gauge field due to disclinations modifies the kinetic term as well. It is clear that this modification will result in principally new situation for the localisation process. A theoretical analysis of dislocated materials showed [5, 6] that the localised electron states always exist (at least with $j = 0$) provided that the deformation potential is the attractive one. This is not the case for topologically unstable disclinations with the fractional Frank index where even for $j = 0$ there exists a compensating positive term in (5) caused by the centrifugal energy. Hence the problem of the electron localisation in this case requires an additional analysis. To proceed further we need the explicit form of the deformation potential.

Let us consider first a disclination with a small Frank index in a cylinder with an inner radius R_c and an external radius R. In this case, the explicit form of the strain tensor was obtained in the form [14, 15]

$$SpE_{AB} = -\frac{\nu(1-2\sigma)}{2(1-\sigma)}\left(2\ln\frac{r}{R} + 1 + \frac{2R_c^2}{R^2-R_c^2}\ln\frac{R_c}{R}\right) \qquad (6)$$

where σ is the Poisson constant. Then the effective potential (5) is written as

$$U_j(r) = \frac{\nu(1-2\sigma)}{2(1-\sigma)}G_d\left(2\ln\frac{r}{R} + 1 + \frac{2R_c^2}{R^2-R_c^2}\ln\frac{R_c}{R}\right) + \frac{(j-\nu)^2\hbar^2}{2m^*r^2} \qquad (7)$$

An exact analytical solution of (3) with the potential (7) is not known yet. A simple qualitative analysis shows that the potential (7) is repulsive for $\nu < 0$ (it corresponds to the positive disclination [14]) and, obviously, the localised electronic states do not appear in this case. On the other hand, for $\nu > 0$ (negative disclination) the effective potential (7) may be the attractive one. This case is of our interest here.

We performed numerical calculations with the wide set of parameters. Physically interesting region in R is $R \sim 10^{-6} - 10^{-5}$cm which corresponds to the mesoscopic structural level of the plastic deformation. As is known (see, e.g. [15]), in crystallites of this size the creation of the small-angle (partial) disclinations becomes energetically preferable in comparison with dislocations of the same geometry. Notice that in this case $R/R_c \sim 10^2$, so that the last term in (6) is negligible. Figure 1 shows (7) for different ν. A depth of the potential well is found to vary over a wide range with the model parameters used. At $\nu = 0.1$ the lowest electron levels are found to be $E_0^{j=0} = -0.66$eV, $E_0^{j=1} = -0.57$eV, $E_1^{j=1} = -0.13$eV, and $E_1^{j=0} = 0.06$eV. At

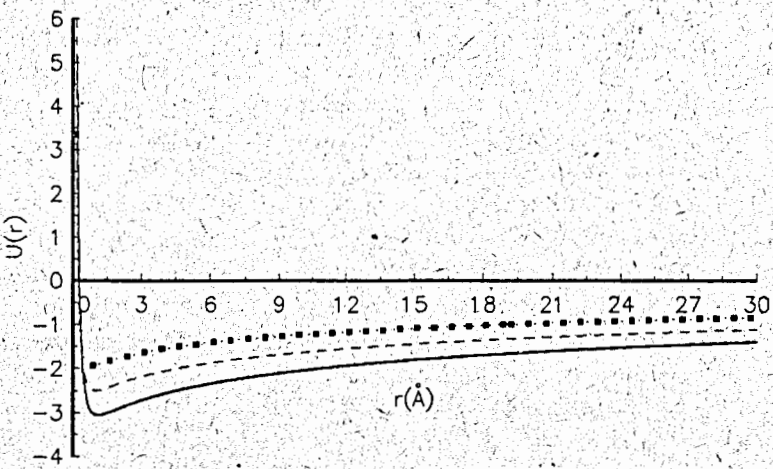

Figure 1. The effective potential (5) (in eV) for the small-angle straight wedge disclination: $\nu = 0.1$ - solid line, $\nu = 0.08$ - dashed line, $\nu = 0.06$ - marked by squares. The parameter set used is: $R = 5 \times 10^{-6}$cm, $m^* = 5 \times 10^4$eV, $G = 10$eV, $\sigma = 0.41, j = 0$.

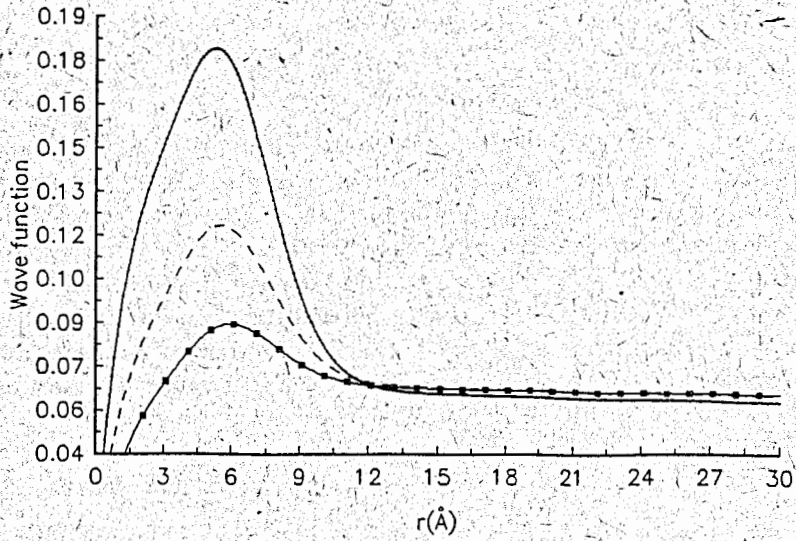

Figure 2. Normalised wave functions of the ground state with $\nu = 0.1$ - solid line, $\nu = 0.08$ - dashed line, $\nu = 0.06$ - marked by squares. The parameter set is the same as in figure 1.

$\nu = 0.08$ $E_0^{j=0} = -0.48$eV whereas at $\nu = 0.06$ $E_0^{j=0} = -0.48$eV. The levels of localised electrons become deeper when the depth of the well increases. The electron wave functions are presented in figure 2. One can see that the amplitude of the localised wave function decreases rapidly with decreasing of ν. The electron states are found to be either strongly localised near the disclination line or become delocalised over the region R.

Strictly speaking, description of strongly localised states is beyond the applicability of the effective mass approximation. That is why the results concerning deep electron levels must be considered only as the qualitative ones. Let us remark, however, that sometimes the use of the effective mass approximation for description of strongly localised electron states (e.g., electrons localised in the core region of a dislocation [16] or electrons localised in the plane, see discussion in [17]) gives even a quantitative agreement with experimental results.

An exact solution for topologically stable linear disclination which corresponds to the complete straight wedge disclination has been found in [13]. It is important to note that this solution contains the information about the core region of the disclination. Namely, we found the explicit form of the deformation potential in a wide space region including the core of a defect. The effective potential was written as follows [7]:

$$U_j(r) = \begin{cases} G_d - DG_d \cosh^2[\frac{1}{3}\cosh^{-1}(r_0/r)] + K(j)/r^2, & r \le r_0 \\ G_d - DG_d \cos^2[\frac{1}{3}\cos^{-1}(r_0/r) + \frac{2}{3}\pi l] + K(j)/r^2, & r \ge r_0 \end{cases} \quad (8)$$

where $D = 4(\lambda+\mu)/3(\lambda+2\mu)$, λ and μ are the Lamé constants, $K(j) = (j-\nu)^2\hbar^2/2m^*$. The point $r = r_0$ in (8) turns out to be the boundary between two regions: the core region where deformations are large, and the region beyond the core where deformations decrease slowly and tend to a constant value at $r \to \infty$. In this paper, we will analyze the case $l = 0$. One can see that for $j = 1$ the potential (8) becomes the attractive one, and, therefore, the discrete levels exist at any set of the model parameters. This conclusion is confirmed by numerical calculations. Figure 3 shows the effective potential for different r_0. The corresponding wave functions are presented in figure 4. At $r_0 = 20$Å the lowest electron level is $E_0^{j=1} = -2.5$eV. For the state with $j = 0$ the localisation takes place as well but with the lower amplitude, and $E_0^{j=0} = -0.62$eV. As r_0 increases, the depth of the potential well rapidly increases and the first electron level becomes remarkably deeper. Conversely, for small r_0 the well is shallow and the lowest level lies close to the edge of the continuum electron spectrum. For $r_0 = 15$Å $E_0^{j=1} = -0.83$eV.

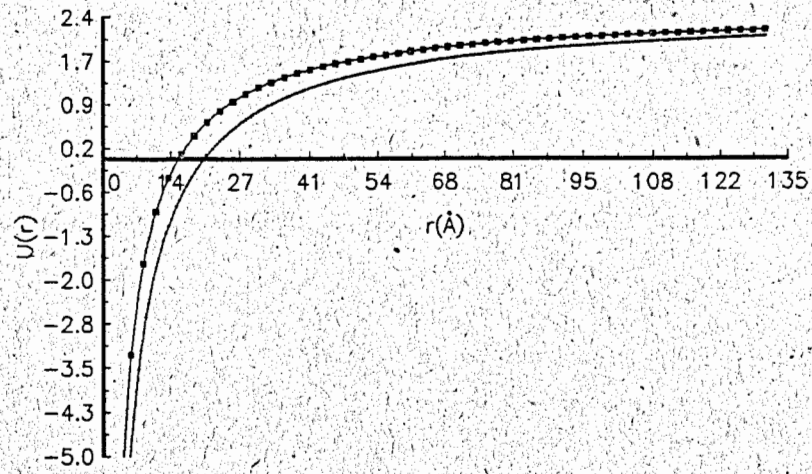

Figure 3. The effective potential (7) (in eV) for the complete straight wedge disclination with $\nu = 1$: $r_0 = 20$Å– solid line, $r_0 = 15$Å– marked by squares. The parameter set used is: $m^* = 5 \times 10^4$eV, $G = 10$eV, $D = 1, j = 1$.

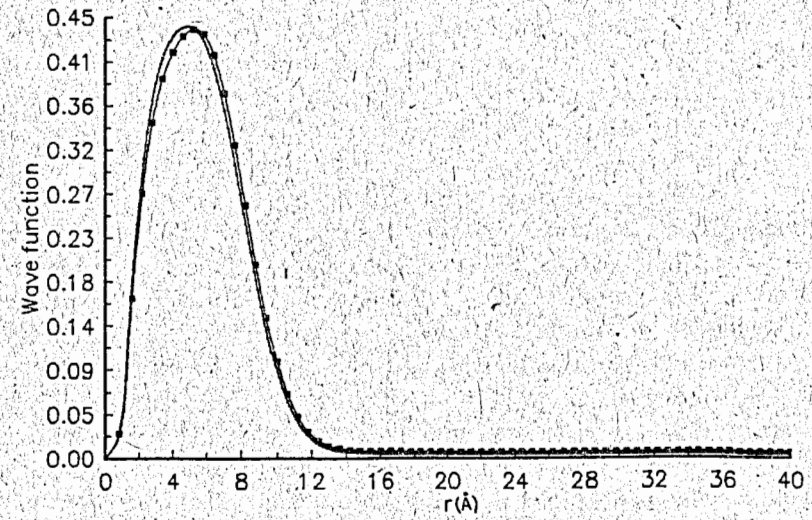

Figure 4. Normalised wave functions of the ground state for the complete straight wedge disclination with $\nu = 1$. Designations and the parameter set are the same as those in figure 3.

Let us consider the point-like disclination with the exact solution [18] called the disclination monopole. The gauge fields W_A were found to be [18]

$$W_A^\alpha(x^B) = \varepsilon_{AB}^\alpha \frac{x^B}{r^2}, \tag{9}$$

Because of the spherical symmetry, the solution of (1) can be chosen in the form $\Psi(x^A) = \Psi(r)\Psi(\theta,\phi)$. Then, for the radial wave function Eq.(1) is written as

$$[\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr} + \frac{2m^*}{\hbar^2}(E - U_j(r))]\Psi_E(r) = 0 \tag{10}$$

where the effective potential takes the form [18]

$$U_j(r) = \begin{cases} (3/2)G_d - BG_d\cosh^2[\frac{1}{3}\cosh^{-1}(r_0/r)^2] + K(J)/r^2, & r \le r_0 \\ (3/2)G_d - BG_d\cos^2[\frac{1}{3}\cos^{-1}(r_0/r)^2 + \frac{2}{3}\pi l] + K(J)/r^2, & r \ge r_0 \end{cases} \tag{11}$$

Here $B = 2(3\lambda + 2\mu)/3(\lambda + 2\mu)$, $K(J) = [J(J+1) - 1/4]\hbar^2/2m^*$, $J = 1/2$ at $j = 0$, $J = j \pm 1/2$ at $j = 1, 2...$ Qualitative analysis showed [19] that a potential well can occur in the core region. For a sufficiently deep well the discrete electron levels and the localised states can appear.

Let us study this problem in detail by solving (10) with the potential (11) numerically. Figure 5 shows the exact form of the wave functions for different r_0. One can see that the localised states really appear but their amplitudes decrease with decreasing of r_0. It should be noted that there is an important difference between the results obtained for the disclination monopole and those for a complete wedge disclination. Namely, as was found above, the localised electron state always exists for the complete wedge disclination, at least for $j = 1$. In the case of the disclination monopole the last term in (11) turns out to be non-zero for any j. Thus the potential well may appear to be too shallow to localize the electron. In fact, the depth of the well is found to be very sensitive to the value of r_0. At $r_0 = 10$Å the lowest electron level is $E_0^{J=1/2} = -3.3$eV whereas at $r_0 = 9$Å $E_0^{J=1/2} = -1.1$eV.

Let us summarize the main results. We showed that the binding of electrons to a small-angle straight wedge disclination take place only for the negative disclination. The amplitude and the position of the localised electron state depend on the depth of the potential well. The first excited state is that with $j = 1$. For the complete straight wedge disclination ($\nu = 1$) the localisation was found to always be present for a state with $j = 1$. In contrast to the small-angle defect, the first excited state in this case is the state with $j = 0$. In both these cases, an electron is free to move along the z-axes. For

a disclination monopole, the localisation takes place only for a sufficiently deep potential well. When this takes place, an electron becomes completely captured by the disclination.

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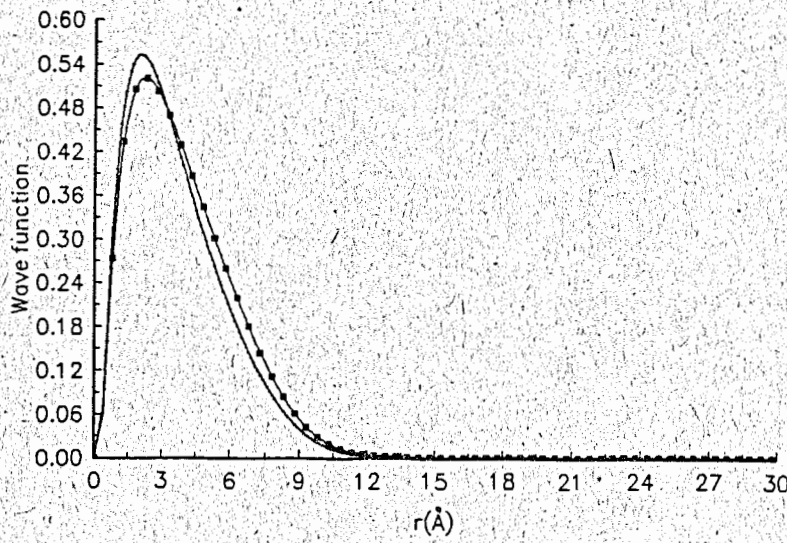

Figure 5. Normalised wave functions of the ground state for the disclination monopole: $r_0 = 10$Å– solid line, $r_0 = 9$Å– marked by squares. The parameter set used is: $m^* = 5 \times 10^4$eV, $G = 6$eV, $B = 1, J = 0.5$.

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