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ON THE INFLUENCE OF THE ELECTRON COMPONENT OF LATTICE DEFORMATION ON LOCALIZED STATES IN CRYSTALS WITH DISLOCATIONS

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Using earlier proposed method of selfconsistent investigation of the lattice strain the localized electron states in the vicinity of an edge staight linear dislocation are analyzed, namely the dependence on the value of the electron-deformation interaction. It is shown that the depth of the state location nonmonotonously depends on such an interaction.
Key words: linear dislocation, electron-deformation interaction, localized electron states.

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It is known that the mechanical distortion of a crystal lattice caused by dislocations,twinning planes and impurities can essentially change its electron properties. The study of these effects is an important aspect of both experimental and theoretical investigations [1–4]. A similar task in a crystal with dislocation was considered in [5]. A dislocation was presented by the δ-like distortion on the axis in its core. For the description of the distortion let us use $U(r) = \mathrm{Sp}U = (\Omega(x) - \Omega_0)/\Omega_0$ (Ω_0 is a crystal cell volume of the undeformed lattice). $U > 0$ corresponds to the lattice extention and $U < 0$ to its shortening. In [1] it is shown that in the $U > 0$ case ($U < 0$) in the electron spectrum the localized splitted out of the bottom (top) of the band states appear. The influence of the potential slowly changing away from the distortion axis on the localized states was investigated in [2, 5]. According to more accurate theory which takes into account electron-deformation interaction [4, 6, 7] the parameter of the lattice deformation essentially depends on the degree of the conduction band population. Below we analyze the electron spectrum of defect crystal with straight linear dislocation in the frame of the model taking into account the electron-deformation interaction. We consider an isotropic metal with a dislocation with an axis along OZ and with a Burger vector b along OX. Then all-round mechanical strain out of the dislocation core region in cylindrical coordinates with polar coordinates (ρ, θ) in XOY plane can be written in the form [8]:

$$\sigma_m(\rho,\theta) = \mathrm{Sp}\widehat{\sigma}_m = -\frac{2|b|}{3\pi}\frac{1+\nu}{1-\nu}C_{66}\frac{\sin\theta}{\rho}, \rho \geq \rho_0 \qquad (1)$$

Where ν is Poisson's coefficient, C_{66} is a metal elastic modulus, ρ_0 is a radius of a dislocation ($\rho = (1-2)a$, a is a crystal parameter). The Hamiltonian of the system in the site representation is:

$$\widehat{H} = \sum_{j\sigma}[W + SU(r_j)]c^+_{i\sigma}c_{i\sigma} + \sum_{ij\sigma}\lambda_{ij}c^+_{i\sigma}c_{j\sigma} + \frac{1}{2}\sum_i C\Omega_0 U^2(r_i) + H_c \qquad (2)$$

Here the 1st term is a Hamiltonian of an electron on the site r_i with taking into account a change of its energy by deformation (S is a constant of deformation potential, W is a reference to the origin of the energy chosen in the middle of the band).The 2nd term is an electron mixing of the i-th and j-th sites in nondeformed crystal; the 3rd one is a potential energy of the elastic deformed crystal (C is an elastic modulus). The 4th term is Coulomb interaction. ($c^+_{i\sigma}, c_{i\sigma}$ are fermion operators). The parameter of the total deformation $U(r)$, caused by mechanical strain $\sigma_m(r_i)$ consists of electron and mechanical components. Outside the region of the dislocation it may be obtained from the condition of the mechanical equilibrium [9]:

$$\left\langle \frac{\partial \widehat{H}}{\partial U} \right\rangle = \sigma_m(r)V \qquad (3)$$

where V is the crystal's volume. Considering (2), condition (3) in momentum representation takes the form of

$$U(r) = -\frac{S}{C\Omega_0}\sum_{kk'\sigma}\langle c^+_{k\sigma}c_{k'\sigma}\rangle \exp[-i(k-k')r] + U_m(r) \qquad (4)$$

where the first term describes the electron component of the total deformation $U(r)$. The mechanical one, $U_m(r)$, as a result of the mechanical strain in cylindrical coordinates is

$$U_m(\rho,\theta,z) = \mathrm{Sp}\widehat{\sigma}_m = -D\frac{\sin\theta}{\rho} \tag{5}$$

with

$$D = \frac{2C_{66}}{3C}\frac{|b|}{\pi}\frac{1+\nu}{1-\nu}.$$

From (4) it follows that the electron component of deformation is accompined by the determination of the $\langle c^{+}_{k\sigma}c_{k'\sigma}\rangle$ correlator which is connected with the electron conduction band concentration

$$n(r) = \sum_m \frac{\psi^*_m(r)\psi_m(r)}{\exp[\beta(\lambda_m-\mu)]+1} \tag{6}$$

by Fourier-transformation. In (6) $\psi_m(r)$ is a solution of Schrodinger equation

$$\left[\nabla^2_r - \frac{S}{\alpha}U(r) + \frac{e}{\alpha}\varphi(r)\right]\psi_m(r) = -\frac{1}{\alpha}\lambda_m\psi_m(r). \tag{7}$$

Here $\alpha = \frac{\hbar^2}{2m}$ (m is an effective mass) and λ_m is an energy counted off λ_0. The last term in the left hand of (7) is the electrostatic energy caused by the charge redistribution. The potential $\varphi(r)$ may be obtain from Poisson equation

$$\nabla^2_{\rho\theta z}\varphi - g^2\varphi = \nabla^2_{\rho\theta z}SU_m = \frac{2DS}{\rho_0^2}\delta(\rho-\rho_0)\sin\theta \tag{8}$$

Here $g = \frac{e}{(R_s/\epsilon\epsilon_0)^{1/2}}$, i.e. it is a value inverse to an effective radius of screening dependent on the band population n, the elastic modulus and the effective mass. Here

$$R_s = \frac{1}{\alpha}\left(\frac{3n_0}{8\Omega_0\pi^4}\right)^{1/3}\frac{\sqrt{1+\left(\frac{n_m}{9\Omega_0\pi^4}\right)^{1/3}\frac{S^2}{\alpha C}}}{1-\frac{3}{2}\frac{S^2}{\alpha C}\left(\frac{n_m}{9\Omega_0\pi^4}\right)^{1/3}\sqrt{1+\left(\frac{n_m}{9\Omega_0\pi^4}\right)^{1/3}\frac{S^2}{\alpha C}}} \tag{9}$$

where

$$n_m = n_0\left[1+\left(\frac{n_m}{9\pi^4}\right)^{1/3}\frac{S^2}{\alpha C}\right]^{3/2} \tag{10}$$

— is an average total concentration of the electron in a crystal in consideration of electron-deformation interaction.

The system of equations (4), (5)–(7) and equation

$$\frac{\Omega_0}{V}\int n(r)dr = \check{n},\ 0 \le \check{n} \le 2 \tag{11}$$

which allows to determine chemical potential were solved in [4, 6, 10] ($\check{n} = n_m\Omega_0$). According to [10] the potential $\varphi(r)$ is

$$\varphi(\rho,\theta,z) = -\frac{2DS}{\rho_0}\sin\theta\begin{cases} K_1(g\rho_0)I_1(g\rho), & \rho\in[0,\rho_0] \\ I_1(g\rho_0)K_1(g\rho), & \rho\in[\rho_0,\infty) \end{cases} \tag{12}$$

where $K_1(g\rho)$ is McDonalds function, and $I_1(g\rho)$ is the first kind Bessel function of the first order [12]. A strain of the crystal in the vicinity of the edge core induced by both its mechanical component $U_m(\rho,\theta)$ and a component originating from the electron redistribution $\triangle n(\rho,\theta,z) = n(\rho,\theta,z) - n_m$ is defined by relation [10]:

$$\triangle U(\rho,\theta,z) = -\frac{S}{C}\triangle n(\rho,\theta,z) + U_m(\rho,\theta) \tag{13}$$

where

$$\triangle n(\rho,\theta,z) = -SR_sD\sin\theta\left[\frac{2}{\rho_0}I_1(g\rho_0)K_1(g\rho) - \frac{1}{\rho}\right]. \tag{14}$$

Note that the analysis (in the frame of quasiclassic approximation) is justifiable for the $\mu a^2 \le 0.01$ case [3] (a is some characteristic length of the problem, f.ex., a lattice parameter). The existence of regions with negative values of the potential $SU(r)$ can be risen to localized states. Analyze such a possibility. As far as the potential of dislocation (5) has a two-dimensional character Schrödinger equation with such a potential is a two-dimensional task. Let $A(E)$ be a region where inequality

$$SU < E \equiv \epsilon - \lambda_0 - \alpha k_z^2 \tag{15}$$

is realized. Define $G(E)$ as a spatial density per unit surface at $SU = 0$. For smoothing a potential well it takes the form of

$$G(E) = \frac{dN}{dE} = \int_{\triangle U<0} G_0(E - SU)dA(E). \quad (16)$$

In the two-dimensional case $E(k_{xy}) = \alpha k_{xy}^2$ and $G_0 = 2\pi m/h^2$. Then

$$\frac{dN}{dE} = \frac{2\pi}{\hbar^2} mA(E) \quad (17)$$

Define the boundary of region $A(E)$. From equality $S \triangle U = E$ and equation (13) we have

$$E = \frac{SD}{\rho}\sin\theta\left[\frac{S^2 R_s}{C}\left(\frac{2\rho}{\rho_0}I_1(g\rho_0)K_1(g\rho) - 1\right) - 1\right]. \quad (18)$$

For the elastic strain at $\rho > \rho_0$

$$K_1(g\rho) = \frac{1}{2g\rho} + 0\big((g\rho)^{-3/2}\big) \quad (19)$$

and E from (18) takes the form of

$$E = \frac{SD}{\rho}(q-1)\sin\theta \quad (20)$$

where

$$q = \frac{S^2 R_s}{C}\frac{\sqrt{\pi}}{g\rho_0}\Big(I_1(g\rho_0) - 1\Big) \quad (21)$$

is a parameter taking into account the influence of the electron-deformation interaction on the level of the electron states localization. In this case

$$A(E) = \int\int \rho d\rho d\theta = \frac{1}{2E^2}S^2 D^2(q-1)^2\int_0^\pi \sin^2\theta \quad (22)$$
$$= \frac{\pi S^2 D^2 (q-1)^2}{4E^2}$$

and (17) in consideration of (20) takes the form of

$$\frac{dN}{dE} = \frac{\pi^2 m S^2 D^2}{2\hbar^2 E^2}(q-1)^2 \quad (23)$$

and

$$E_N = -\frac{\pi^2 m S^2 D^2 (q-1)^2}{2\hbar^2}\frac{1}{N}, \quad N = 1, 2, 3\ldots \quad (24)$$

From (24) it follows that localized states behave as a $\sim N^{-1}$ decreasing sequence. It coinsides with the results of [5].

From (24) the conclusions follow that

- for "weak" electron-deformation interaction, $q \in [0, 1]$,the localized states are closer to the band bottom than in the case of such an interaction. If q tends both from the right and from the left to one, E tends to the band bottom;
- for the "large" q, $q > 2$, or its negative value (such a situation at certain correlations between n_m, S, C, m according to (9), (21) is possible) localized states are depeer and the absolute value q increasingly tends to lower such states.

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ПРО ВПЛИВ ЕЛЕКТРОННОЇ СКЛАДОВОЇ ДЕФОРМАЦІЇ ҐРАТКИ НА ЛОКАЛІЗОВАНІ СТАНИ В КРИСТАЛАХ З ДИСЛОКАЦІЯМИ

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Отримані раніше результати самоузгодженого розрахунку деформації ґратки застосовуються до аналізу електронних локалізованих станів в околі крайової прямолінійної дислокації. Проаналізована поведінка цих станів залежно від величини електрон–деформаційної взаємодії. Показано, що ступінь залягання локалізованих рівнів немонотонно залежить від величини такої взаємодії.