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ELECTRON PAIRING MEDIATED BY NANODISTURBANCES IN HIGH-T_C SUPERCONDUCTORS

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Abstract. A special mechanism of electron pairing in superconducting cuprates is suggested. The mechanism is based on the electron-electron interaction mediated by quasistable nanodisturbances, planar nanoscopic areas of local shear with tiny shear vectors. Structural factors are discussed which enhance formation of nanodisturbances in superconducting cuprates.

High-transition-temperature (T_c) superconductivity in cuprates represents the subject of intensive research efforts; see, e.g., reviews [1-3]. Of crucial interest is the mechanism of electron pairing responsible for high-T_c superconductivity in these advanced materials. At present, though there are many experimentally documented facts and theoretical models concerning electron pairing, its nature is still an open problem; see, e.g., [1-10]. This situation is related to the complexity of the high-T_c superconductivity phenomenon which may be based on two or more mechanisms for electron pairing. In particular, several research groups reported on experimental data indicative of the important role of atomic motions in high-T_c superconductivity; see, e.g., [10-13]. In this context, one can consider the conventional electron-phonon interaction (responsible for the elecron pairing in conventional high-T_c superconductors) as a mechanism capable of contributing to electron pairing in cuprates. At the same time, with the specific features (e.g., d-symmetry of electron wave functions, an unusual isotope effect, dramatic suppression of critical current by grain boundaries) of superconducting cuprates, the standard representations on electron-phonon interaction are questionable in description of high-T_c superconductivity. This motivates interest in at least modification of these representations (see, e.g., [4,14,15]) and/or even search for a new mechanism of elecron pairing, which is related to atomic motions. In recent years, a special type of crystal lattice excitations – nanodisturbances - has been experimentally revealed [16-19] and theoretically described [19-21] in solids. Nanodisturbances by definition [19-21] represent planar nanoscopic areas of local shear with tiny shear vectors. The main aim of this Letter is to suggest a new mechanism of elecron pairing related to atomic motions – the namely pairing through formation of nanodisturbances – in high-T_c superconducting cuprates. Because of both the complexity of the problem and the original description [19-21] of nanodisturbances in terms of micromechanics of defects, we will use semiclassical approach in our further consideration of elecron pairing mediated by nanodisturbances.

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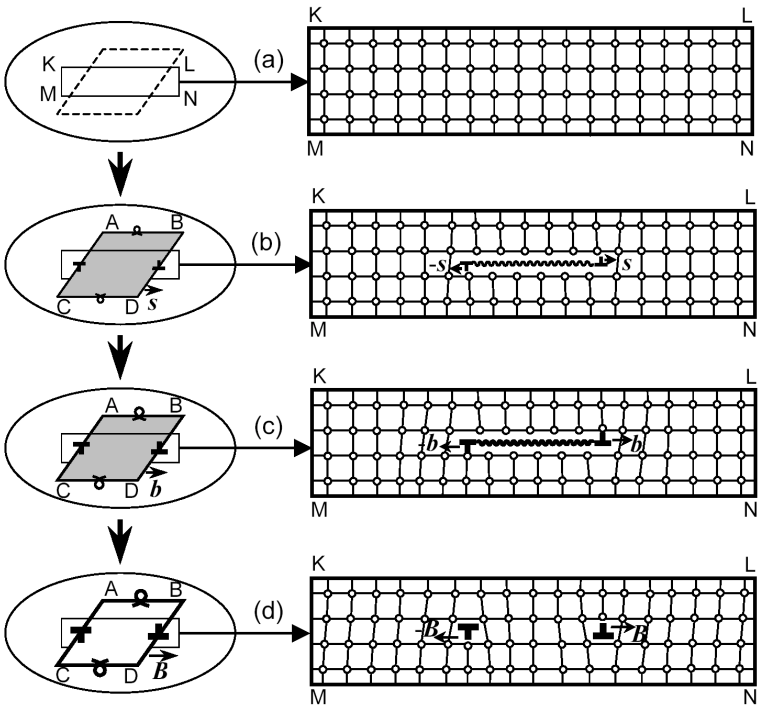

Fig. 1. Generation of nanodisturbance and its transformation into perfect dislocation loop in crystalline solid. (a) Initial, defect-free state. (b) Generation of nanodisturbance - planar nanoscopic area ABCD where local tiny shear occurs - under an external shear stress. The nanodisturbance is bounded by loop of 'non-crystallographic' partial dislocation with small Burgers vector ***s*** . A generalized stacking fault (separating two parts of the crystal lattice that are slightly sheared by vector ***s*** relative each other at the nanoscale area) is formed within the area ABCD. (c) Shear increases along the area ABCD that contains the generalized stacking fault. Shear is characterized by vector ***b*** serving as Burgers vector of the corresponding partial dislocation loop. (d) Vector characterizing shear along the area ABCD reaches the lattice vector ***B***. In this case, partial dislocation loop transforms into perfect dislocation loop, and generalized stacking fault within the area ABCD disappears. General view is shown on the left parts of figures (a)-(d). The magnified insets on the right parts of figures (a)-(d) highlight (in terms of crystal lattice transformations) generation and evolution of nanodisturbance in rectangular area KLMN that intersects nanodisturbance ABCD. Generalized stacking fault is shown as wavy lines on the right parts of figures (b) and (c).

First, let us discuss the notion of nanodisturbances defined [19-21] as planar nanoscopic areas of local shear with tiny shear vectors (Figs. 1a and 1b). Each nanodisturbance is bounded by loop of non-crystallographic partial dislocation with small Burgers vector characterizing tiny shear occurring within nanodisturbance (Fig. 1b). Nanodisturbances were experimentally observed by high resolution electron microscopy in Gum Metals, a newely discovered group of titanium alloys with specific properties [16-19]. Within the theoretical approach, nanodisturbances were defined and described as defects whose evolution under the mechanical stress results in formation of lattice (partial or perfect) dislocations in Gum Metals [19] and nanomaterials [20,21], as shown in Fig. 1. In doing so, evolution of a nanodisturbance occurs through increase (from 0) of the Burgers vector magnitude, while geometric sizes of the nanodisturbance either are constant or weakly change during the evolution (Fig. 1). Very recently, Cui, *et al*. [18] have reported on "in situ" experimental observation (by high resolution electron microscopy) of transformations of nanodisturbances into lattice dislocations in titanium alloys, corresponding to the scheme shown in Fig. 1. Note that the specific feature of nanodisturbances is their non-local formation in which a cooperative movement of a group of atoms within a nanoscale area is involved (Figs. 1a and 1b).

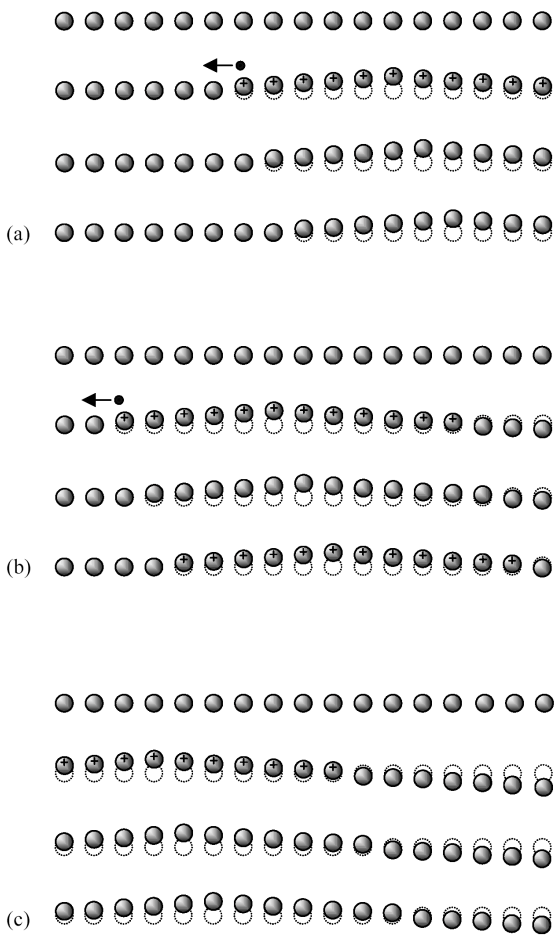

Fig. 2. Crystal lattice vibrations are induced by electron movement in ionic lattice (schematically). When the electron (small full circle) moves along a crystallographic plane in vicinity of ions, they slightly move towards the electron. As a result, the moving electron excites both vibrations of the crystal lattice and corresponding charge polarization in local regions. For simplicity, vibrations of the crystal lattice fragment located "above" the moving electron are not shown.

Now let us turn to a semiclassical description [22] of electron pairing mediated by crystal lattice vibrations in conventional superconductors. For illustration, we schematically consider electron-movement-induced vibrations of a simple cubic crystal lattice consisting of positively charged ions. Let an electron move along one of crystallographic planes of the lattice (Fig. 2). When the electron moves in vicinity of ions, they slightly move towards the electron, as schematically shown in Fig. 2. In doing so, the moving electron excites both vibrations of the crystal lattice and corresponding charge polarization in local regions. In particular, a region with some extra positive charge is formed, for a short time period, in the wake of the moving electron (Figs. 2b and 2c). The positively charged local area can attract another electron [22]. This attraction allows the electrons to form pairs that carry electric current in superconductors at temperatures lower than critical temperature T_c. Thus, wihin the semiclassical description, the electron pairing is mediated by crystal lattice vibrations in conventional low-T_c superconductors [22]. In the framework of quantum mechanics of crystalline solids, crystal lattice vibrations are described in terms of phonons, the quanta of such vibrations, while electron pairing is mediated by phonons; for details, see, e.g., [23].

We think that, besides crystal lattice vibrations, nanodisturbances can be excited by electron movement in high-*T*c superconductors. In this case, movement of an electron causes ions to be displaced (from their eqilibrium positions) into quasistable positions within a nanoscale region, and the combined effects of these displacements result in a tiny shear along the nanoscale region or, in other terms, formation of a quasistable nanodisturbance (Fig. 3).

Let us discuss the structural factors that favor electron-movement-induced formation of quasistable nanodisturbances in superconducting cuprates. The common structural factors for superconducting cuprates are the existence of CuO_2 planes and the presence of oxygen vacancies [24,25]. First of all, CuO_2 planes exist in superconducting cuprates, and these planes are separated by intermediate layers consiting of other complicately arranged atomic configurations [24,25]. The equilibrium interatomic distances in the intermediate layers do not coincide with those in CuO_2 planes, in which case there is a spatially inhomogeneous geometric mismatch between atomic arrangements in CuO_2 planes and the intermediate layers [25]. The spatially inhomogeneous mismatch serves as the origin of local strains and deviations in atomic positions from those of the average crystallographic structure of supercoducting cuprates [25]. Besides, superconducting cuprates contain oxygen vacancies creating both similar deviations and local elastic strains. Thus, due to the presence of oxygen vacancies as well as the geometric mismatch between CuO_2 planes and intermediate layers, local elastic strains and deviations in atomic positions from those of the average crystallographic structure typically exist in superconducting cuprates.

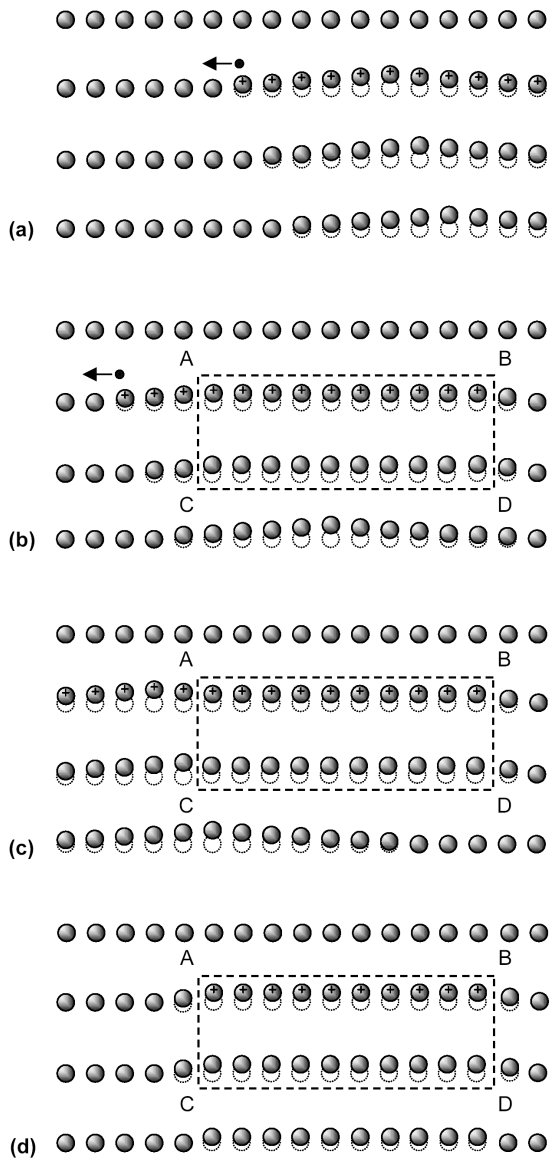

Fig. 3. Electron movement in ionic lattice induces a tiny shear of the ideal structure within nanoscale region ABCD (schematically). More precisely, as a result of movement of electron (small full circle) in ionic lattice, the structure of a superconducting cuprate is transformed within a nanoscale region through group displacements of ions from their ideal positions to new quasistable positions corresponding to a tiny shear within the nanoscale region ABCD. The resultant distorted atomic arrangement in nanoscale region ABCD represents a nanodisturbance.

With the aforesaid local strains and deviations in atomic positions taken into account, we think that, in parallel with the "ideal" atomic configurations having the lowest energy, there are metastable

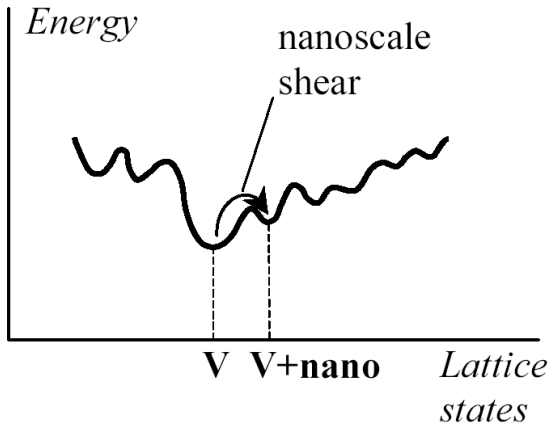

Fig. 4. In parallel with the vacuum atomic configuration (V) having the lowest energy in cuprate lattice, there are metastable atomic configurations separated from the vacuum-state energy by barriers. In particular, shear within a nanoscale area (nanoscale shear) can transform the initial vacuum state (V) into a metastable state of lattice with a nanodisturbance (V + nano).

nanoscale atomic configurations in cuprates. The metastable configurations correspond to energy minimums separated from the vacuum-state energy by barriers (Fig. 4). Each of these metastable nanoscale atomic configurations results from a tiny shear (first of all, shear along a CuO_2 plane) of the ideal structure within a nanoscale region (Fig. 3). In other words, the structure of a superconducting cuprate can be transformed within a nanoscale region through group displacements of ions from their ideal positions to new positions corresponding to a tiny shear within this nanoscale region (Fig. 3). In particular, such displacements can be induced by moving electrons (Fig. 3). The resultant distorted atomic arrangement in nanoscale region ABCD (Fig. 3) is very smilar to nanodisturbances (which are specified by tiny shears within nanoscale regions [19-21] and experimentally observed [16-19] in titanium alloys).

The structural changes under discussion (Fig. 3) are essentially nanoscale in the sense that a resultant atomic configuration is metastable, only if the corresponding shear (induced by electron movement) occurs within a nanoscale region. In this context, the nanoscale structural changes are different from individual jumps of atoms into new quasistable positions. Also, the nanoscale structural changes are different from global structural changes/instabilities which are initiated by variations in the chemi-

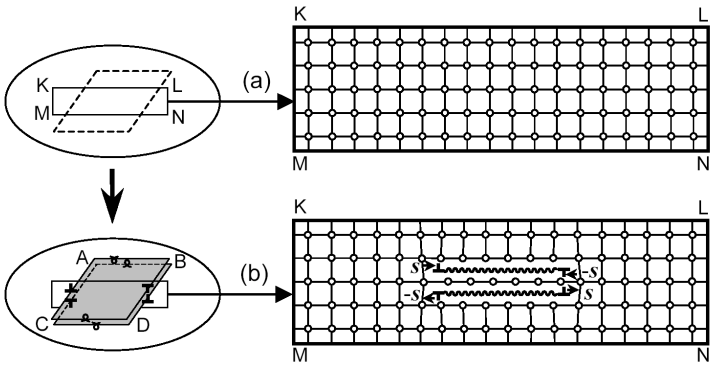

Fig. 5. Generation of nanodisturbance due to electron movement. (a) Initial state. (b) Nanodisturbance ABCD is generated due to movement of a point-like electron. General view is shown on the left parts of figures (a) and (b). The nanodistrbance is bounded by two nanoscale loops of 'non-crystallographic' partial dislocations. The magnified insets on the right parts of figures (a) and (b) highlight (in terms of crystal lattice transformations) generation of nanodisturbance in rectangular area KLMN that intersects nanodisturbance. The nanodisturbance represents one atomic layer (having nanoscale length and width) slightly sheared relative to the neighboring material. The layer is separated from the neighboring material by two generalized stacking faults shown as wavy lines on the right part of figure (b).

cal composition of a cuprate specimen and/or temperature. (A typical example of global structural changes is the orthorhombic-to-tetragonal transformation initiated by variations in oxygen vacancy concentration in YBaCuO and other high-T_c superconductors [4,24].) That is, the system under consideration transfers to a new metastable state (Fig. 4), only if a cooperative shear transformation of group of ions occurs within a nanoscale region (Fig. 3).

The statement on the nanoscale structural changes in cuprate lattices is in an agreement with experimental data [26] showing rather intense X-ray diffuse non-phonon scattering from LaSrCuO single crystals. More precisely, X-ray diffuse scattering was found to be dominated by phonon scattering at room temperature, while residual non-phonon scattering was clearly seen at low temperatures [26]. Also, there are experimental data indirectly indicating in favor of the suggested representations on nanoscale structural transformations in cuprates. For instance, it was experimentally found that cores of lattice dislocations composing low-angle grain boundaries with certain geometric parameters in YBaCuO split into nanoscale cylinder-like regions having the disordered structure [27]. These nanoscale lattice transformations are effectively described as those induced by local stresses existing in the vicinities of dislocation cores in YBaCuO [28]. In this context, one expects that cuprate lattices tend to undergo nanoscale structural transformations, and the idea on formation of nanodisturbances in superconducting cuprates is rather natural. In addition, lattice dislocations with nanoscale cylinder-like cores, similar to those in cuprates, were experimentally observed in Gum Metals (see experimental data [16] and a theoretical model [29]), titanium alloys where nanodisturbances were experimentally found to exist [16-19].

Thus, with the presence of oxygen vacancies as well as the geometric mismatch between CuO_2 planes and intermediate layers, the cuprate crystal lattice energy is expected to have, in parallel with its vacuum state energy minimum, minima corresponding to metastable states of the lattice (Fig. 4). Group displacements of ions – in particular, those induced by moving electrons – can transfer a portion of ions into new quasistable positions within a nanoscale region (Fig. 3). The resultant distorted atomic arrangement in the nanoscale region ABCD (Fig. 3) is very smilar to nanodisturbances (specified by tiny shears within nanoscale regions) experimentally observed in titanium alloys [16-19]. At the same time, there is a difference in geometry between stress-induced nanodisturbances (Fig. 1) in Gum Metals and (hypothetical) electron-movement-induced nanodisturbances (Fig. 3) in cuprates. A stress-induced nanodisturbance is bounded by

one dislocation loop (Fig. 1), because it separates two parts of the crystal lattice that are slightly sheared relative each other at the nanoscale area. A nanodisturbance induced by movement of a point-like electron, in fact, represents one atomic layer (with nanoscale length and width) slightly sheared relative to the neighboring material. Therefore, such a nanodistrbance is bounded by two nanoscale dislocation loops, as schematically shown in Fig. 5.

After some time interval, the ions can return to their "ideal" positions from quasistable ones with the aid thermal fluctuations, and the nanodisturbance decays. Lifetime t_{nano} of the nanodisturbance depends on both temperature and the energy barrier between the vacuum state and the state with a nanodisturbance (Fig. 4). Note that a quasistable nanodisturbance represents a defect whose metastability is due to the stabilizing effect of spatially inhomogeneous geometric mismatch between atomic arrangements in CuO_2 planes and the intermediate layers within a nanoscale area. In this context, nanodistrbances are different from polarons (that may contribute to electron pairing in cuprates [30]), because atomic displacements associated with polarons are stabilized by the presence of charge carriers.

To summarize, a special mechanism is suggested which is capable of contributing to the electron pairing in high-T_c superconducting cuprates. The mechanism is based on the electron-electron interaction mediated by nanodisturbances, planar nanoscopic areas of local shear with tiny shear vectors. Within the suggested approach, moving electrons induce formation of quasistable nanodisturbances (Fig. 3) and corresponding charge polarization in nanoscale regions, which is responsible for electron pairing. Such structural factors as the existence of CuO_2 planes and the presence of oxygen vacancies enhance formation of nanodisturbances in superconducting cuprates. In doing so, the structural changes associated with formation of nanodisturbances (Fig. 3) are essentially nanoscale in the sense that a resultant atomic configuration is metastable, only if the corresponding shear (induced by electron movement) occurs within a nanoscale region. In this context, the nanoscale structural changes are different from both individual jumps of atoms into new quasistable positions and global structural changes like the orthorhombic-to-tetragonal transformation. The discussed statement on the nanoscale structural changes in cuprate lattices is in an agreement with experimental data [26] showing rather intense X-ray diffuse non-phonon scattering from LaSrCuO single crystals.

Finally, this Letter was concerned with only a qualitative description of the electron pairing mediated by quasistable nanodisturbances in high-T_c superconducting cuprates. Further theoretical and experimental studies are worth being carried out for identification of nanodisturbances and their potential role in high-T_c superconducting cuprates.

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