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Thermodynamically equilibrium point defects in the low-dimensional systems

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The temperature dependencies of the electrical resistance of low-dimensional $NbSe_3$- and $NbSe_2$-single crystals were investigated in the range of 300–540 K. Measurements of resistance were produced along the chains for quasi-one-dimensional $NbSe_3$-single crystal and along the layer for quasi-two-dimensional $NbSe_2$-single crystal. On the temperature dependencies the exponential deviations from linear dependencies were observed. We suppose that such deviations of resistance are connected with the contribution of selenium equilibrium vacancies.

Key words: *low-dimensional systems, electroresistance, vacancies*

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Numerous experimental and theoretical works [1,2] are devoted to a research of properties of low-dimensional conducting systems. Due to a reduced dimensionality, such compounds have got an anisotropy of physical properties, in particular anisotropy of conductivity ($\rho_\perp/\rho_{//}$=10–20 at $NbSe_3$ [3]; $\rho_\perp/\rho_{//}$=30–50 at $NbSe_2$ [2]) and at the same time the role of thermodynamic fluctuations increase. It is known that conductivity hardly depends on concentration of defects. Magnitude of concentration of the defects is determined by the significance of the bond energy and by co-ordination of atoms in the crystal lattice. The $NbSe_3$ and $NbSe_2$ researched in the present work are typical representatives of quasi-one-dimensional and quasi-two-dimensional compounds. The compounds of $NbSe_3$ and $NbSe_2$ consist of identical atoms but they differ by space co-ordination of atoms. For this reason these compounds were selected as the objects of a comparative experimental research of vacancy formation processes. The present work is devoted to experimental study of temperature dependence of a resistance as well as the processes of formation of thermodynamically equilibrium dot defects (monovacancies) in $NbSe_2$ and $NbSe_3$.

Crystals of $NbSe_3$ and $NbSe_2$ were prepared using gas transport reaction [4]. Quasi-one-dimensional single crystals $NbSe_3$ [1] consist of a chain formed by trigonal prisms from Se atoms (figure 1a). At the centre of such prisms the Nb atom is located. The bond between the chain is weak. It leads to a quasi-one-dimensionality of this

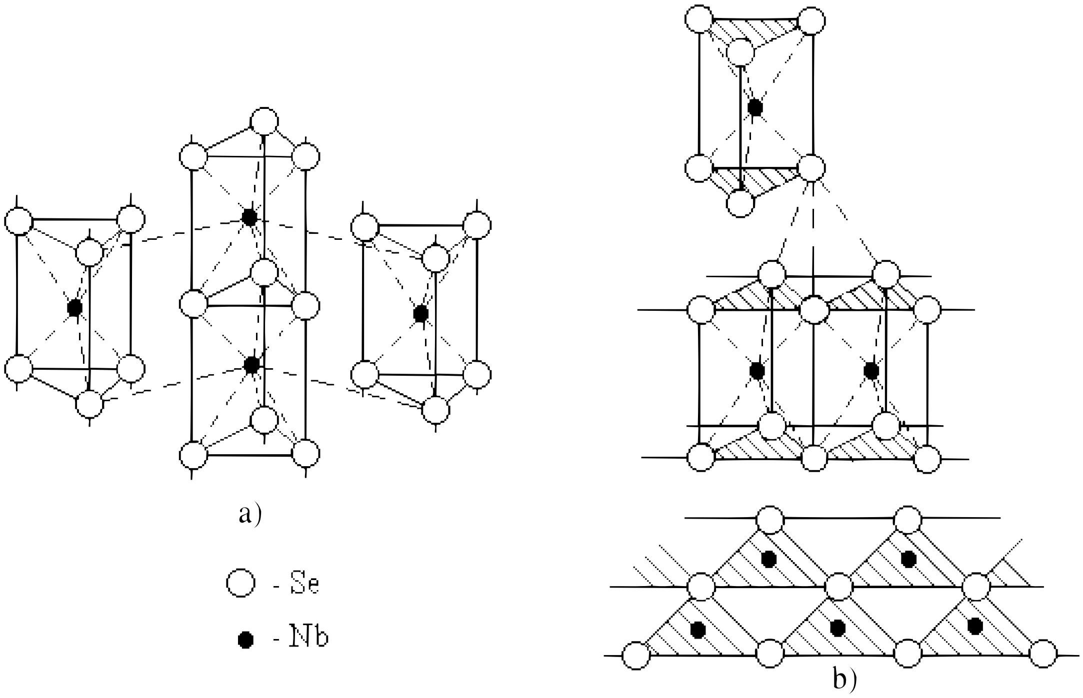

Figure 1. Structures of single crystals of quasi-one-dimensional NbSe3 (a) and quasi-two-dimensional NbSe2 (b).

compound. The number of the nearest bonds for atom Se (disregarding the bonds between chains) is equal to six (4 of them are Se-Se bonds, 2 are Nb-Se bonds). The atom of Nb has 6 nearest Nb-Se bonds and 2 Nb-Nb bonds.

Quasi-two-dimensional single crystals $NbSe_2$ [2] consist of layers, each of which represents a sandwich from two layers of atoms Se with a layer Nb between them (figure 1a). The layers $NbSe_2$ interact among themselves in the crystal by weak Van-der-Vaals forces. Coordination number for Se is 9 (6 bonds of Se-Se and 3 bonds of Nb-Se). At the atom Nb there are 6 Nb-Se bonds and 6 Nb-Nb bonds. As the number of bonds for atoms Se, both at $NbSe_2$, and at $NbSe_3$, is less than for Nb, the energy of vacancy formation of atoms Se is less than the energy of vacancy formation of atoms Nb. The ratio of the number of the nearest bonds for atoms Se in compounds $NbSe_2$ and $NbSe_3$ is 9:6. Thus, it is possible to assume that the energy of vacancy formation of atoms Se in $NbSe_2$ should be approximately 1.5 times higher than at $NbSe_3$, the energy of vacancy formation of atoms Nb being approximately equal.

The temperature dependencies of the electroresistance of single crystals in low-dimensional systems $NbSe_3$ and $NbSe_2$ were investigated in the region of temperatures higher than 300 K. The electroresistance was measured using a four-contact DC circuit along the chains for a quasi-one-dimensional $NbSe_3$-single crystal and along the layer for a quasi-two-dimensional $NbSe_2$-single crystal. The transport current value was such that the electric field at the sample was lower than the threshold electric field of charge density wave sliding [1].

The temperature dependence of electroresistance of samples $NbSe_3$ and $NbSe_2$ in

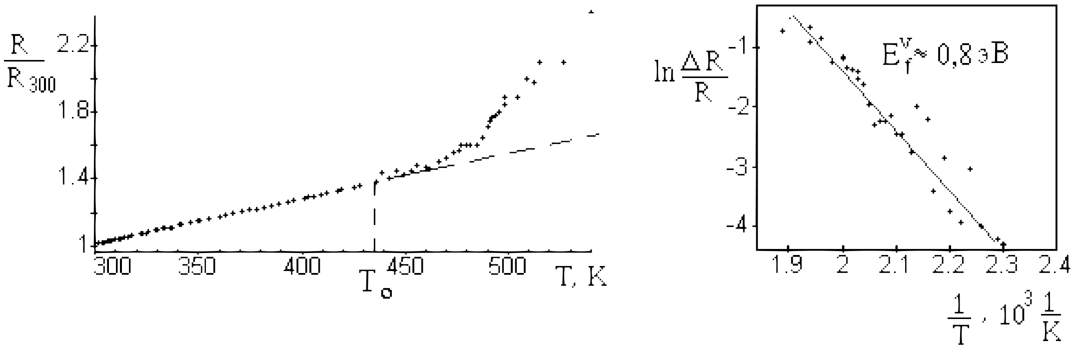

Figure 2. Temperature dependence of electroresistance NbSe3 (a) and activation energy (b).

the temperature interval of 300–540 K is presented in figures 2a and 3a accordingly.

The obtained temperature dependencies of electroresistance for both single crystals $NbSe_2$, and for $NbSe_3$ show the deviations from the linear dependence at $T>T_o$. In case of well-investigated three-dimensional metals [5], the similar deviations from the linearity are stimulated by forming thermodynamically equilibrium vacancies. In our case of low-dimensional systems, the observable effects are also stimulated by forming thermodynamically equilibrium vacancies. The definition of magnitudes of activation energies is represented in figures 2b and 3b in coordinates $\ln(\Delta R/R) = f(1/T)$ (ΔR – residual between experimental and exponential value of resistance at the temperature T). For $NbSe_3$ the magnitude of energy of activation E_f^v has made up 0.8 eV (the same result is obtained in the experiment made in vacuum), for $NbSe_2$ E_f^v=1.2 eV.

Taking into account the results obtained ($E_f^v(NbSe_2) \approx (1{,}5 E_f^v\ (NbSe_3))$ we consider the vacancies in $NbSe_2$ and $NbSe_3$ -single crystals to be the vacancies of Se. However in low-dimensional systems the formation vacancy may lead to breaking the lattice stability. It is a possible reason of nonrepeatability of experimental results on different samples.

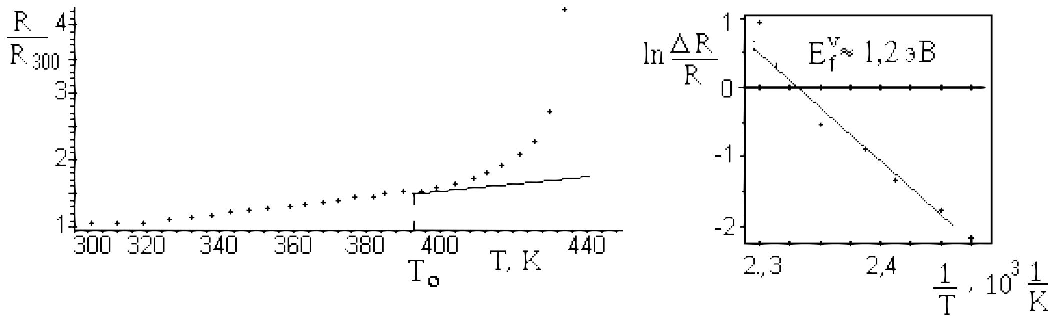

Figure 3. Temperature dependence of electroresistance NbSe2 (a) and activation energy (b).

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Термодинамічно рівноважні точкові дефекти в низькорозмірних системах

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Досліджено температурні залежності електричного опору низькорозмірних монокристалів $NbSe_3$ та $NbSe_2$ в температурному діапазоні 300–540 K. Вимірювання опору виконувалися вздовж ланцюжків для квазіодномірних монокристалів $NbSe_3$ та вздовж шарів для квазідвомірних монокристалів $NbSe_2$. На температурних залежностях опору виявлені експоненційні відхилення від лінійної залежності. Припускається, що ці відхилення пов'язані з внесками від рівноважних вакансій селену.

Ключові слова: *низькорозмірні системи, опір, вакансії*

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