

MODELLING OF ELECTRICAL CONDUCTIVITY OF SOME QUASI-ONE-DIMENSIONAL ORGANIC CRYSTALS

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Organic crystals attract more and more attention as materials with much more diverse and often unusual properties. Among such crystals the quasi-one-dimensional ones present a particular interest due to sophisticated structure determined by the chainlike stacking of molecules.

Some quasi-one-dimensional organic crystals are distinguished by especially high room electrical conductivity $\sigma(300)$ along the chains and very strong temperature dependence $\sigma(T)$ with a sharp peak ratio of $\sigma(T_m)/\sigma(300)$, where $\sigma(T_m)$ is the value of electrical conductivity at the temperature T_m , when the maximum is achieved. For example, in the TTF-TCNQ (tetrathiofulvalene-tetracyanoquinodimethane) crystals this peak ratio is of the order of several tens and is very sensitive to crystals purity. However, in spite of many experimental and theoretical publications, the transport properties of such crystals are not yet completely understood. It is explained by multiple interaction mechanisms involved. Presently, the mentioned behavior of electrical conductivity is interpreted as the contribution of sliding charge density waves.

In this paper we propose another interpretation of the temperature dependence of electrical conductivity, based on the crystal model, developed in [1, 2]. One considers that the overlap of electronic wave functions along the chains is great, determining a band-like transport mechanism. Between the chains the wave function overlap is small and the transport mechanism in the transversal to chains direction is hopping-like. In the first approximation one neglects the small contribution to electrical conductivity from the hopping carriers motion and one obtains a one-dimensional crystal model. The latter is described in the tight binding and nearest neighbors approximations. The conduction electrons are moving along the chains into a one-dimensional conduction band.

The model takes into account simultaneously two interaction mechanisms of conduction electrons with acoustical lattice vibrations. One mechanism is deformation potential similar and is determined by the variations, due to thermal vibrations, of the transfer energy (transfer integrals) of an electron from a molecule to the nearest one along the chain. Only the conduction band width is rather small, because the overlap of molecular orbitals is relatively small even along the highly conducting chains. Therefore, the variation of electron and phonon quasi-momentums is taken on the whole Brillouin zone. The second mechanism is polaron similar, only the question is about the induced polarization. So as the crystal molecules are big, they are highly polarizable. The conduction electron polarizes surrounding molecules and interacts with the induced dipoles. The same acoustic thermal vibrations displace the molecules leading to large variation of the polarization energy.

Under certain conditions the interference between these two interactions becomes possible, and they considerably compensate each other for some definite states into the conduction band. As a result, the inclusion of the second interaction does not diminish, but increases the electrical conductivity and determines other peculiarities of transport properties. In a large temperature interval the scattering processes can be considered elastic. In this case the kinetic equation is solved exactly and the relaxation time of carriers can be introduced. Due to mentioned interference, the relaxation time as a function of carrier energy has a form of Lorentzian, which, under certain conditions, can have a rather high maximum. This means that the carriers with the energy around the maximum will have increased mobility, and the crystal will be characterized by high room electrical conductivity.

For electrical conductivity an analytical expression is obtained which contains a transport integral as a function of carrier energy. The electrical conductivity is modeled in dependence of temperature for different crystal parameters. Very high maximums are obtained which can exceed the room value by more than two orders of magnitude. Here we present also the comparison of electrical conductivity modeling with experimental data for TTF-TCNQ crystals in a large temperature interval. It is shown that the considered model describes rather well the temperature dependence of electrical conductivity, including high peaks and abrupt decrease after peaks.

References

1. A. Casian et. al., Phys. Rev. B 66, 165404 (2002).
2. A. Casian et. al., Phys. Low-Dim. Str., 9/10, 43 (2002).