Symbolic and Numerical Calculation of Transport Integrals for Some Organic Crystals

A. Casian[1], R. Dusciac[1], V. Dusciac[1], and V. Patsiuk[2]

[1] Technical University of Moldova, Av. Stefan cel Mare, 168, MD-2004 Chisinau, Rep. of Moldova
[2] State University of Moldova, Str. A. Mateevici, 60, MD-2009 Chisinau, Rep. of Moldova

Abstract. The kinetic integral equation for a quasi-one-dimensional organic crystal is solved exactly, and the expression for the electrical conductivity is presented as a transport integral. The latter has two singularities depending on crystal parameters. The possibilities to obtain analytic expressions in some particular cases and the general numerical calculations with pronounced singularities are analysed.

1 Introduction

Organic materials attract more and more attention of investigators as low cost replacements for conventional metals and inorganic semiconductors and as materials with much more diverse and often unusual physical properties [1]. These materials are now widely used as the active elements of organic-based devices such as light-emitting diodes and lasers for displays, photovoltaic cells, field-effect transistors, and real-time holographic optical recording and processing systems [2, 3, 4, 5]. Unusual high electrical conductivity [6, 7] and the thermoelectric efficiencies [8, 9, 10, 11] are also predicted in a special class of quasi-one-dimensional (Q1D) organic crystals under certain conditions. However, in spite of a great number of theoretical and experimental publications in this field, the mechanism of charge transport in organic materials is not completely understood yet. This is connected, on the one hand, with a rather large and diverse number of transport mechanisms in these materials, and on the other hand, each mechanism is more complicated than in ordinary inorganic materials.

We have studied a model of Q1D organic crystal which takes into account simultaneously two main interactions of conduction electrons with acoustic vibrations of crystalline lattice [6, 7], and also the scattering on impurities and defects. The first interaction is similar to deformation potential and is caused by the variation of the transfer energy of an electron from a molecule to the nearest one. The other interaction is polaron similar and is determined by the variation of the polarization energy of molecules surrounding the conduction electron. These interactions have been studied in the literature [12, 13, 14]. But we have considered these two interactions for the first time together in Q1D crystals. This is important because under certain conditions the interference between

V.G. Ganzha, E.W. Mayr, and E.V. Vorozhtsov (Eds.): CASC 2006, LNCS 4194, pp. 101–108, 2006.