Calculation of the electron effective mass in a nanodiamond-metal composite

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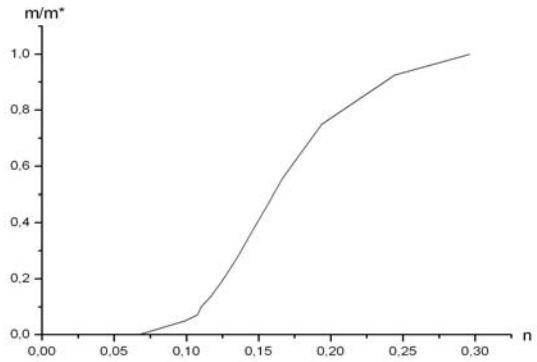
Under investigation is a material in which the diamond nanoparticles are immersed in the metal. The effective mass of electron m of such materials is essentially depends on sizes and mutual location of the differently conducting regions. In order to understand in workmanlike manner the available regularities, it is solved the problem with a periodic structure. Diamond nanoparticles will be considered to be the same size d and immersed in the metal at the same distances L. Nanoparticles make up a cubic lattice.

Calculation is made by the well known kp-method. Diamond nanoparticles influence on m is introduced by the local electron-phonon interaction potential in form of Gaussian function with maximum value U0~0,1eV [1]. The Schrödinger equation with corresponding potential is solved by means of the Fourier transformation, which gives the system of linear equations. So received Wave functions, received in that way, are used for calculation of effective mass [2].



The dependence of inverse effective mass on the concentration is shown on the diagram. This diagram shows that in the area of applicability of the theory effective electron mass increases with increasing concentration of diamond nanoparticles and therefore, for example, the electrical conduction of the nanodiamond-metal composite is changed non monotonically. Experimental detection of this effect would confirm the correctness of the choice of such a potential of electron-phonon interaction. Of course, in a real sample effect will be less expressed because of the disorder.

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