

Nanocomposites and nanomaterials

Electrons in the intercalated stage ordered layered structures: Description by the periodic Anderson model

I.V. Stasyuk, O.V. Velychko

Institute for Condensed Matter Physics of the National Academy of Sciences of Ukraine, 1 Svientsitskii Str., 79011 Lviv, Ukraine

Changes in the electronic band structure of the layered nanohybrid compound of the GaSe-type with a stage ordering (three layers in the packet in the considered case) due to intercalation are studied within the model which is a simplified version of the periodic Anderson model. We have considered two cases: the single-level model and the single-level model with damping effects (which widen the level). The principal restructuring of the electron spectrum and the respective density of states consists in additional splitting, emergence of gap (or pseudogap) and appearance of the single impurity band besides the main one. Being far enough from the main band, the impurity band degenerates into the impurity level. Approaching each other they hybridize with reconstruction of the respective edge of the main band.

In the case, when the single-electron energy spectrum of the impurity particle is approximated by the density of states of the Lorentzian shape, the smearing out of the full spectral density takes place. At the increase of parameter that characterizes the local level broadening degree, the singularities of the total density of states (DOS) gradually smear out, the hybridization gap in the energy spectrum disappears, and the three-step structure of density of states near the energy band edge becomes less distinctive. Similar changes in the DOS take place at the increase of the intercalant concentration [1].

Knowledge of the total density of states allows one to calculate the electron quantum capacitance of the considered intercalated layered compounds [2]. In the low temperature limit the frequency dispersion of the DOS determines the field (voltage) dependence of the quantum capacitance, which strongly depends on localization of impurity bands, strength of electron hybridization and temperature.

1. Grygorchak I.I., Kostrobiiy P.P., Stasyuk I.V., Tokarchuk M.V., Velychko O.V., Ivashchyshyn F.O., Markovych B.M. Physical processes and their microscopic models in periodic inorganic/organic clathrates. – Lviv, Rastr-7, 2015 – 285 p. (in Ukrainian).
2. Stasyuk I.V., Velychko O.V. Electron spectrum of intercalated stage ordered layered structures: Periodic Anderson model approach // Mathematical Modeling and Computing. – 2015. – 2, N. 2. – P. 191–203.