FIZIKA 6 (1974) 113—116

LETTER TO THE EDITOR

PECULIARITIES OF THE FORMING OF THE LOCAL ONE-ELECTRON LEVELS SYSTEM IN AN IMPERFECT CRYSTAL

V. N. SALOMOTOV and I. A. PARFIANOVICH

Irkutsk State University, Irkutsk, USSR

Received 1 April 1974

Abstract: Green's function method developed by Lifshitz[1] for solving of local perturbation problems, was successfully applied for vibrational states investigation of crystals with defects[2]. Investigation of the electron states by this method, Koster's and Slater's paper[3] being the beginning, was carried out mainly on model systems[4-6]. Obvious possibilities of this method for calculations of concrete crystals with impurities was mentioned in the review[7].

Nowadays the local one-electron levels in KCL-T1[8], KCl-Eu[10-12] as well as in semiconductors with impurities[13-14] were calculated by the Green's function method. The results of the calculations turned out to be interesting for the interpretation of the experiment[10-14]. Level sets with different magnitude of perturbation parameters were compared with the purpose of studying of the local states nature in KCl-Eu[12]. The further calculation number increase for the concrete electron systems should be expected. Thus the exposure of this method application peculiarities for the electron problem solution seems to be useful.

In the Green's function method local levels arise in the energy gap by the turning into zero of the one-electron energy E function

$$f(E) = \det|\hat{I}_d - \hat{G}_d\hat{U}_d|, \tag{1}$$

where $\hat{I}$ is a unit operator, $\hat{G} = (E\hat{I} - \hat{H})^{-1}$ is a resolvent operator ($\hat{H}$ is the Hamiltonian of the ideal crystal), $\hat{U}$ describes the perturbation introduced by the defect. The mark d means that the operator is localized in the limited defect range of a crystal.

Study of the influence of the different perturbation parameters (inducing, own-impure and mixing[9]) on the local one-electron levels system in KCl-Eu allows to reveal two kinds of levels that differ from each other in the character of dependence of their position and existence on perturbation parameters.

Levels which position monotonously change with the change of correspondence parameters (after the emergence with some critical quantity of parameters) are related to the first type (I). E. g. levels having inducing nature[12] arise from the valence band and with the decrease (the absolute quantity being increased) of the inducing parameters move down the energy axis. Each of these levels can arise and vanish with all the other local levels preserved.

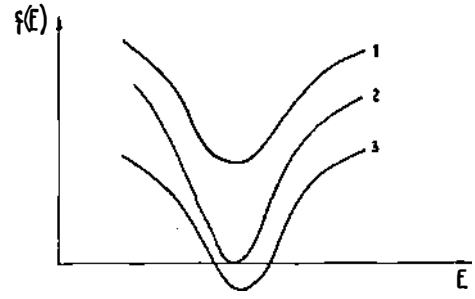

Fig. I I- type levels appearance; 1, 2, 3- determinant $f(E)$ with three different magnitudes of perturbation parameters.

Levels of the second type (II) arise and vanish in pairs i. e. with the monotonous change of some group of perturbation parameters mutual rise and then disappearance of two levels at once is observed. The rise of the second-type levels is qualitatively illustrated in the figure. Most frequently the I I- type levels arise when impurity one-electron energies in the crystal (impure parameters) approach to the valence band. E. g. in the KCl-Eu crystal in the case of excited state of impurity ion there are I I- type local levels with E = — 0.36 eV (the energy being counted from the valence band bottom). The distance between these levels is less than 0.01 eV. It became possible to discover them only by the study of the local levels system dependence on the perturbation parameters. Near from each other situated I I- type levels peculiarity, is their strong position dependence (in comparison with the I-type levels) on the perturbation parameters. These levels can arise and vanish

with the small perturbation parameters changes, in the process of arising and vanishing »degeneracy points« being observed (case 2 in the Figure). Equations

$$f(E_1) = 0;\ f(E_2) = 0; \tag{2}$$

$$\left.\frac{df}{dE}\right|_{E=E_0} = 0,\ E_1 < E_0 < E_2,$$

are conditions of the levels E_1 and E_2 appearance in pair.

The study of these equations was carried out in the simplified two-band model of the one-atom crystal with a cubic lattice, one atom of which being replaced by an impurity atom. As it turned out the second-type levels do not arise with the change of a single perturbation parameter (all the rest being equal to zero). Realization of equations (2) becomes possible if two perturbation parameters (as minimum) take part in local levels system formation. Therefore it is possible to say that the I I- type levels rise is conditioned by the »interaction« of the different perturbation parameters in the forming of the local one-electron system in the crystal with a defect.

By the practical realisation of the Green's function method determinant $f(E)$ is usually calculated in the band gap with some step ΔE. The local level rise is determined by the $f(E)$ mark change in the ΔE interval. Pair levels with energies E_1 and E_2 can be not discovered if $(E_1 - E_2) < \Delta E$.

Taking into account this circumstance as well as the fact that pair levels position and existence depend strongly on perturbation parameters, the whole row of simplifying approximations being introduced in each concrete calculation, it seems to be necessary to calculate not only the $f(E)$ function but also the $\frac{df}{dE}$ function. In the energy range near to the point, where $\frac{df}{dE}$ turns to zero, one should not only decrease ΔE but also carry out additional investigation of the $f(E)$ function dependence on the perturbation parameters as well as on the number of considered parameters.

References

1) И. М. Лифшиц, ЖЭТФ **17** (1947) 1017; **17** (1947) 1947) 1076; **18** (1948) 293;
2) A. A. Maradudin, Theoretical and Experimental Aspects of the Effects of Point Defects and Disorder on the Vibrations of Crystals, Academic Press Inc., New York-London, 1966);
3) G. Koster and J. Slater, Phys. Rev. **95** (1954) 1167; **96** (1954) 1208;
4) J. Callaway, J. Math. Phys. **5** (1964) 783;
5) J. Callaway and A. Hughes, Phys. Rev. **156** (1967) 860;
6) N. Kristoffel and G. Zavt, Nuovo Cim. **61B** (1969) 331;

7) Н. Н. Кристофель, Труды ИФФА АН ЭССР, **32** (1967) 97;
8) N. N. Kristoffel, G. S. Zavt and B. V. Shulichenko, Physics of Impurity Centres in Crystals Tallinn (1973) 53;
9) Н. Кристофель, В. Саломатов, Изв. АН ЭССР, физ.-мат., **21** (1972) 245; Preprint FAI-14, Tartu, 1972;
10) В. Саломатов, Н. Кристофель, Изв. АН ЭССР, фмз.-мат., **21** (1972) 337;
11) И. А. Парфианович, В. М. Мецик, В. Н. Саломатов, Е. И. Ширалева, Оптика и спекроскопия **35** (1973) 876;
12) В. Н. Саломатов, Н. Н. Крисмофель, Материалы XXI Совещания по люминеценции (крисмаллофосфдры), Ставрополы (1973) 133; Изв. АН. СССР, сер. физ. (в. печати);
13) R. A. Faulkner, Phys. Rev. **175** (1968) 991;
14) A. Baldereschi, J. Luminescence **7** (1973) 79.