Comparison of Thermodynamic Functions for Different Models of Electron Spectrum in Layered Crystals

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Abstract – **Different models of electron energy for *GaSe* are considered to deriving the thermodynamic functions of electron gas at low and high temperatures. Their common features and differences are pointed out and their agreement with existing data is analyzed. The results allow to find out the cases where different models produce the similar results and to analyze the conditions where the peculiarities of chemical bonding are to be considered.**

Keywords – **Thermodynamic functions, Layered crystals.**

I. INTRODUCTION

Layered semiconductors (LS) are wide used in photoelectronic and electronic devices. Due to intercalation, performed on these crystals they are attractive for energy store and hydrogen energy devices. These crystals have peculiarities of chemical binding, which manifest their particular one-particle spectrum. We consider two wide used models of electron spectrum in our investigations. For Fivaz' model we analyze the dependences of thermodynamic functions on parameter, which is essentially affected by intercalation, as well as the transition from closed to opened surfaces.

II. QUASI-CLASSICAL ELECTRON GAS

This approximation means low concentrations of electrons and high (room) temperatures of the semiconductor. In this paper two wide used models of electron spectrum are used: the parabolic and Fivaz [1] dispersions. Thermodynamic functions are evaluated, using expressions, based on statistical sums. Expression for statistical sum for Fivaz model was developed in [2]. We investigated the analytical expressions for thermodynamic functions using Fivas one-particle approximation, analyzed their temperature dependences and compared them with well known dependences for parabolic gas with *GaSe* parameters. Comparing these datas for temperature range 250 K - 550 K we conclude: a) electron gas energy shows very close values for both dependences; b) specific heat differs a little bit stronger for this temperature range and show a relative divergence within the range 1,7 % for 250 K and 5,1 % for 550 K; c) the thermodynamic potentials differ essentially – almost for the whole temperature range we observe about 30% increase of its absolute value for parabolic spectrum (typical of isotropic semiconductors) – this differences can be explained by the chemical binding in layered semiconductors; but both functions show nearly the same increase with temperature:

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d) entropy shows anomalously small differences for both models (about $1{,}1\cdot10^{-4}$% at 250 K). This enable us to conclude that the dependences of thermodynamic functions on temperatures are quite similar for both models as long as we deal with quasi-classical gas.

III. FERMI ELECTRON GAS

This approximation is used in a case of low temperatures and high concentrations of electrons. We used the inverse Laplace transform in [3] to define the density of states. It differs essentially from the obtained for parabolic dispersion. Besides, in the case of Fivas dispersion and high concentrations of particle it does not depend on the temperature. These results explain the anomalous increase of absorption coefficient for some frequencies, received in [4] for *GaSe*. For Fivaz dispersion the small region of specific parameters is found with negative volume expansion coefficient. This agrees with he results of [5], where the negative value of the linear expansion coefficient is shown and explained by bend waves, which are typical of phonon spectra of layered crystals. But in [6] it was shown that bend wave for *GaSe* does not exist. This effect appeared due to Fivaz dispersion and can also take place for phonon system. In the case of Fivaz dispersion we found the entropy independent on electron concentration for opened energy surfaces at some parameters. This conclusion agrees with the results developed for two dimentional cases.

REFERENCES

[1] Fivas R.F., Mosser E, " Electron – phonon interaction in semiconducting layer structures" *Phys. Rev*. vol. 136, №3, pp. 833-836, 1964.

[2] Tovstyuk C.C."Thermodynamical Values of Electron Gas in Layered Crystals" *Molec. Phys. Reports*. vol. 23, pp. 197-199, 1999.

[3] Tovstyuk C. "Thermodynamic functions of an electron gas in strongly anisotropic crystals for different models of electron spectrum" *Chem. of Metals and Alloys*. Vol.4, pp.58-62, 2011.

[4] Захарук А.П. Терехова С.В., Тодоров С.М. "Край полосы поглощения GaSe" *Физ. Техн. Полупр.*т. 10, № 12, сс.. 2367 – 2370, 1976.

[5] Belenkii G.L., et al. "The nature of negative linear expansion in layered crystals C, BN, GaS, GaSe, and InSe", *Sol. St. Communs*, vol. 53, No. 11, pp. 967 – 971, 1985.

[6] Jandl. S., Brebner J.L., Levy F. "Lattice dynamics of GaSe" *Phys. Rev*., vol. B13, № 2, pp. 686 – 693, 1976.