OSCILLATIONS OF KINETIC COEFFICIENTS OF SEMIMETALS

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SUMMARY

An expression for the Fermi level displacement upon appearance of a disbalance between the carriers of electron and hole type is deduced. A model of two subsystems of carriers is suggested, which explains the experimentally detected temperature and impurity concentration anomalies of kinetic coefficients of semimetals.

1. INTRODUCTION

The kinetic features of semimetals preserve mainly the characteristics of metal properties, namely, rather high carrier densities, low electronic heat capacity, and nonzero conductivity at T = 0. However, they have many properties similar to those of semiconductors, namely, the change of signs of the Hall constant and thermopower, which are determined by the specific type of their conductivity. Therefore, semimetals appear to be sensitive to the energetic characteristics of scattering centers, which makes them close to semiconductors.

The tendency of bismuth crystal lattice to the substitution by atoms of the fourth (Sn, Pb) and sixth (Se, Te) groups indicates the charge disbalance of lattice impurities.

This circumstance was used by us to explain the experimentally detected "oscillations" of the kinetic characteristics of the semimetals (Bi) with impurity concentration [1]. In this paper, we note the specific role of substitution impurity in semimetals containing at least two atoms per elementary cell. This circumstance is reflected experimentally as "oscillation" of kinetic coefficients at a change in impurity concentration.

Extensive experimental studies [2-4] pointed to the occurrence of temperature oscillations of kinetic coefficients of semimetals. In paper [4], the effect of the thermopower sign inversion is explained to be due to the redistribution of p-type carriers (holes) between one light L_s and two heavy T or $\sum$ bands. The difference in the density of states of effective masses of these bands allows us to explain the sign inversion due to alternation of light or heavy holes in kinetic characteristics. This is in agreement with the theoretical description of thermopower; however, the reason of the alternately turn on of different hole bands is not clear as yet. According to [3], the abnormal behavior of the thermopower temperature dependence is due to a special mechanism of carrier scattering. We agree with this conclusion and focus our attention on the model of the thermopower sign inversion at the resonance scattering of carriers of both types - electrons and holes. In fact, the experimental

studies in the well-known pseudogap model [5] for semimetals with overlapping electron and hole bands confirm the theoretical predictions. This model describes the thermopower sign inversion due to a change in carrier compensation level [8].

2. THE EFFECT OF THE CARRIER DISBALANCE AT FERMI LEVEL DISPLACEMENT

The electron-hole conductivity of semimetals pointed to two subsystems of carriers and a band structure with overlapping energetic bands.

If we make a comparison between the hole states of semimetals and semiconductors, we will see that the occurrence of hole states in the gapless case is special. In contrast to proper semiconductors, where the position of Fermi level (Fermi energy- ξ) is weakly temperature dependent, in semimetals the Fermi level position has a significant temperature dependence due to the difference of carrier effective masses for heavy holes (m_p) and light electrons (m_e) [7]

$$\xi(T)= (\varepsilon_v+ \varepsilon_c)/2+3/4*kTln(m_p/m_e) . \quad (1)$$

The coexistence of hole and electron carriers in a material without a gap is possible due to the charge non-compensation in various points of elementary cell volume. The elementary cell contains at least two atoms in different points of symmetry, which create their own charge surroundings.

Theoretically, each of the subsystems has its own kinetic characteristics. However, in the experiments the cumulative effect takes place. Thus, for the electron subsystem the feature of electron concentration in the conduction band is the Fermi energy of the subsystem, the interrelation of which with concentration is well known [7]

$$n=A_n(kT)^{3/2}*exp[(\xi_n-\varepsilon_c)/kT],$$

where ε_c is the energy of the conduction band bottom, Sn is the Fermi energy that determines the occupation level of the conduction band. The value of A_n depends on another significant feature of carriers, their effective mass

$$A_n= 2* [m_n/2\pi h^2)]^{3/2} .$$

The subsystem of hole carriers has analogous characteristics.

The hole concentration in the valence band is determined by the interrelation:

$$p=A_p(kT)^{3/2}*exp[(\varepsilon_v-\zeta_p)/kT],$$

where ε_v and ζ_p are the energies of the top of the valence band and of the Fermi level of the hole subsystem, the latter determines the occupation level of the valence band. The energies ζ_n and ζ_p depend on filling numbers n and p of respective states in the subsystem bands. The position of the Fermi level $\zeta(T)$ for the system of the arithmetic mean of the Fermi energies of electron and hole subsystems

$$\zeta(T)=(\zeta_n+\zeta_p)/2=(\varepsilon_c+\varepsilon_v)/2+3/4*kTln(m_p/m_n)+kT/2*ln(n/p). \quad (2)$$

In contrast to formula (1), formula (2) for the energy of the Fermi level of a gapless material with electron-hole conductivity can describe the Fermi energy dependence on carrier disbalance. The disbalance is typical for semimetals with electron and hole bands displaced in κ space from k=0 point.

We note that bismuth (Bi) is the one of the most thoroughly studied materials having a system of displaced electron and hole bands [8].

Certainly, in the case of direct bands or charge compensated samples the electric neutrality is provided with the condition n = p, and then formula (2) coincides with formula (1).

However, it should be noted that in this case there exists one more condition for the appearance of a gap between electron and hole subsystems (pseudogap). A special role in the temperature displacement of the Fermi level energy is played by the phenomenon of the carrier localization. At nonzero temperature the carrier concentrations in the bands are determined not only by proper carriers but also by temperature excitation of resonance states of localization. The increase in temperature, in the first place, causes a change in carrier concentration and, subsequently, according to (2), the Fermi level displacements.

3. CONCLUSIONS

The changes in the number of carriers in subsystems depend on temperature and determine the appearance of a negative "pseudogap" and different directions. The sign inversion of the kinetic characteristics of the material by the displacements of the Fermi level depends on the symmetry properties of the material crystal structure. As it was mentioned in [1], the periodicity of the sign inversion of the kinetic characteristics of semimetals depends on the presence of at least two atoms in the elementary cell. The ability of the lattice to localize carriers of different types depends on properties of the charge surrounding these atoms.

The conditions of saturation of localized states or of complete delocalization of one type of carriers are manifested by the change in the Fermi level displacement direction and by the "oscillations" of values of the kinetics coefficients, such as the Hall constant or thermopower. The abnormal dependences of thermopower on temperature and impurity concentration in Bi-Se and Bi-Sn alloys are plotted in Figs. 1 and 2, respectively.

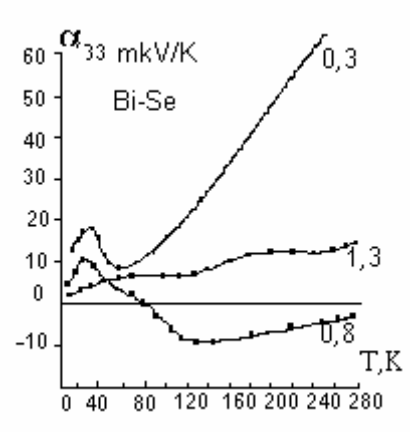

Fig. 1. Temperature dependences of thermopower in Bi-Se alloys for different Se concentrations.

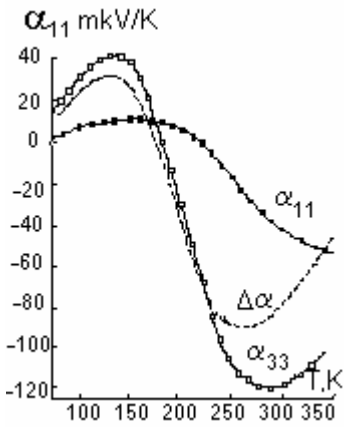

Fig. 2. Temperature dependence of $\Delta\alpha = \alpha_{33} - \alpha_{11}$ of the alloy Bi-0.3 at % Sn.

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