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The cause of anomaly of temperature dependence of electroresistance of the ordering nonstoichiometric FeCo compounds based on a b.c.c. lattice

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ABSTRACT

A theory of energy spectrum and electrical conductivity, which takes into account the electron scattering by the potentials of ions and fluctuations of both the spin and charge densities of electrons in disordered substitutional alloys, is developed. Calculations of temperature–concentration dependence of electrical resistance were performed for b.c.c.-$Fe_{1-c}Co_c$ alloys. The causes of weak temperature dependence of electrical resistance of the Fe–Co alloys are governed by the presence of a quasi-gap in the electron-energy spectrum, which appears due to strong electron correlations as well as atomic and magnetic orders.

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1. Introduction

The Fe–Co alloys possess the unique magnetic and electrical properties conditioned by the presence of strong electron–electron correlations. Strong Coulomb interaction between electrons leads to the formation of a quasi-gap in their energy spectrum. Herewith, the location of the Fermi level within the quasi-gap region is concerned with the appearance of the spin-transport effect and record high saturation magnetization in these alloys [1,2]. In a given work, causes of anomalously weak temperature dependence of the electrical resistance for the disordered $Fe_{0.5}Co_{0.5}$ and $Fe_{0.88}Co_{0.12}$ alloys (for instance, quenched from elevated temperatures) at the temperatures up to 300 K [3] resulting from the location of the Fermi level within the quasi-gap region are investigated.

2. The theory and numerical calculations

For the description of electron states in a crystal, the multiband model of a tight binding and the method developed in Refs. [1,2,4] for the cluster expansion for one- and two-particle Green's functions and thermodynamic potential of the electrons' and phonons' systems of a disordered alloy are used. Within the mentioned method, the coherent potential approximation [5] is chosen as a zeroth-order one-site approximation. This approach allows taking into account the electron scattering by ion potentials of different kinds and fluctuations of both the spin and charge densities with an allowance for correlations in the atom arrangement and orientation of the localized magnetic moments at the lattice sites. The matrix elements of Hamiltonian were calculated within the scope of the Slater–Koster method of linear combination of atomic orbitals in combination with the Löwdin orthogonalization procedure [6–8]. The exact expression for the static electrical conductivity of an alloy, $\sigma_{\alpha\beta}$, is derived in Ref. [1] as follows:

$$\sigma_{\alpha\beta} = -\frac{e^2\hbar}{4\pi N\Omega_0}\int_{-\infty}^{\infty} d\varepsilon \left(-\frac{\partial f}{\partial \varepsilon}\right) Sp \times \left\langle \upsilon_\alpha(G(\varepsilon^+) - G(\varepsilon^-))\upsilon_\beta(G(\varepsilon^+) - G(\varepsilon^-))\right\rangle . \quad (1)$$

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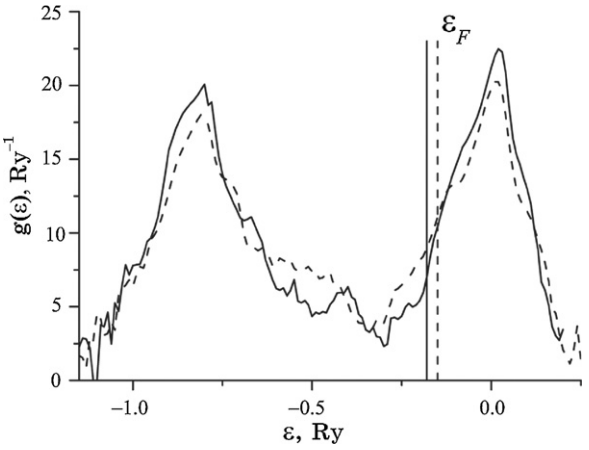

Fig. 1. The electron density of states of the disordered $Fe_{0.5}Co_{0.5}$ (- - -) and $Fe_{0.88}Co_{0.12}$ (—) alloys with account for the electron–phonon interaction at $T = 300$ K.

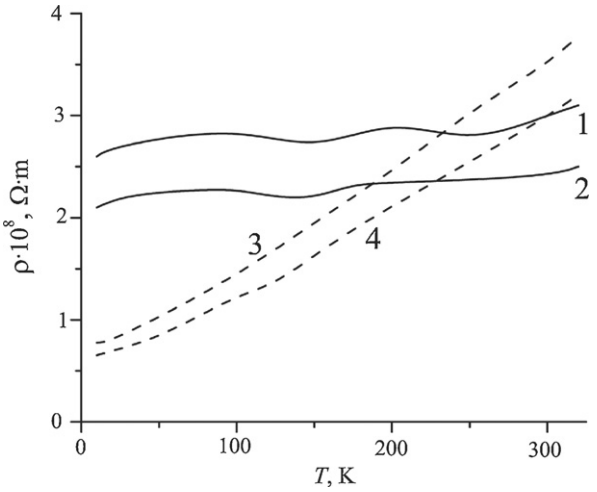

Fig. 2. The temperature dependence of electrical resistance, $\rho = 1/\sigma_{zz}$, calculated by the exact formula (1) (—) and with the expression of the weak-scattering approximation [5] (- - -). Curves 1, 3 refer to dependences at issue for $Fe_{0.88}Co_{0.12}$ alloy, and curves 2, 4—for $Fe_{0.5}Co_{0.5}$ alloy. These computations correspond to Fe–Co alloys (after quenching from elevated temperatures $\leq$1200 K) in a metastable state with achieved equilibrium short-range order.

Here $G(\varepsilon^{\pm}) \equiv G(\varepsilon \pm i\delta) = (\varepsilon^{\pm} - H)^{-1}$, $G = \tilde{G} + \tilde{G}\widehat{T}\tilde{G}$, $G(\varepsilon^{\pm})$ are the retarded ('+') and advanced ('−') Green's functions of a system, H—the one-electron Hamiltonian of an alloy, ε—the energy parameter, $\delta \to +0$; $\tilde{G}$—the Green's function for the effective medium, $\widehat{T}$—the matrix of electron scattering by the random potential; υ_{α}—the α-component operator of the electron velocity vector, $f(\varepsilon)$—the Fermi function; Ω_0—the primitive unit-cell volume; N—the total number of lattice sites; e—the electron charge; $\hbar$—Planck's constant; the brackets $\langle \cdots \rangle$ denote the configuration averaging.

The calculations of both the electrons' energy spectrum and the temperature dependence of static electrical conductivity of the disordered $Fe_{0.5}Co_{0.5}$ and $Fe_{0.88}Co_{0.12}$ alloys based on a b.c.c. lattice are performed. In the course of numerical calculations, the processes of electron scattering by clusters consisting of two scattering centers has been taken into account within the cluster expansion for the scattering $\widehat{T}$-matrix. That allowed to consider an influence of the parameters of atomic and magnetic pair-wise correlations on the electron density of states and electrical conductivity of alloys. Equilibrium values of both the projection of localized magnetic moments and parameters of the magnetic and atomic correlations are obtained from conditions that the free energy is minimum [4]. As revealed, in absence of long-range atomic order, the maximal short-range atomic order is energetically advantageous for the $Fe_{0.5}Co_{0.5}$ alloy as well as for the nonstoichiometric $Fe_{0.88}Co_{0.12}$ alloy. Besides, these compositions are characterized by the short-range magnetic-order parameter closed to its maximal value in ferromagnetic state.

The weak temperature dependence of electrical conductivity of $Fe_{1-c}Co_c$ alloys is caused by the location of the Fermi level within the quasi-gap region in the electrons' energy spectrum that occurs for investigated alloys (Fig. 1). The expression for electrical conductivity, σ, within the weak-scattering approximation, where $\sigma \propto g(\varepsilon_F)\tau$ [5] ($g(\varepsilon_F)$—the electron density of states per one atom at Fermi level, τ—the time of attenuation of electron states) is knowingly not appropriable for the systems with strong electron–electron correlations. However, it allows explaining qualitatively the change of the electrical conductivity due to selection of contributions from the changes of two factors: the electrons' energy spectrum and attenuation of electron states. When the temperature rises up to 300 K, the electrons attenuation time decreases, and the electron density of states at Fermi level increases due to effect of 'tailing' of an energy quasi-gap at scattering of electrons by vibrations of a crystal lattice and due to magnetic disordering of alloys. The competition of mentioned contributions in the electrical-conductivity behaviour leads to their partial compensation. However, the comparison of calculation results for the electrical conductivity, $\sigma_{\alpha\beta}$, by means of the exact expression (1) and the formula within the weak-scattering approximation shows that more intricate temperature dependence of electrical resistance takes place at $T \in$ 0–300 K (Fig. 2).

The results of computations for $Fe_{1-c}Co_c$ alloys conforms qualitatively to the experimental data [3,9,10]. Nevertheless, the experimental values of electrical resistance of these alloys are approximately three times as much the theoretical values. It may be explained by the concentration heterogeneity of investigated alloys and their multiphase states [11] that were not included at the numerical computations.

The expression within the weak-scattering approximation gives the monotonous increase of electrical resistance with the temperature rise (Fig. 2, curves 3, 4), while, calculations by the exact formula (1) give the weak nonmonotonous dependence (Fig. 2, curves 1, 2). The cause of the weak temperature dependence of electrical resistance of disordered phase of b.c.c.-$Fe_{1-c}Co_c$ alloys (with lattice parameters $a \cong 2.85$–2.86 Å [10]), in addition to above-mentioned competing factors, is also the presence of strong electron–electron correlations in a system. The values of localized magnetic moments and parameters of the pair-wise magnetic correlations decrease with the temperature increase that leads to the additional increasing of the electron density of states at Fermi level.

3. Conclusion

The weak change of electrical resistance of b.c.c. $Fe_{1-c}Co_c$ alloys in a metastable (short-range-ordered) state with the temperature increase from 0 K up to 300 K is caused by not only a competition of the contributions concerned with the decrease of attenuation time of electron states and the increase of electron density of states at Fermi level, but also by the effects conditioned by the strong correlations between electrons.

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