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Multipolar interactions in rare-earth metals and alloys

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The Hamiltonian of the indirect quadrupole–quadrupole interaction of rare-earth ions in metals and alloys is constructed self-consistently, taking into account the exchange interactions and correlations in a system of conduction electrons (CE) and the antishielding effects. The manifestations of the indirect multipolar interactions of paramagnetic ions in the parameters of ESR on localized moments in metals and alloys are studied.

During recent years, experimental evidence was obtained for necessity to take into account the multipolar pair interactions to explain the temperature variation of the electric field gradient at the impurity sites in rare-earth metals and alloys [1], and the results of measurements of elastic constant, parastriction and magnetic susceptibility of rare-earth intermetallic compounds [2], and the temperature variation of the anisotropy of the magnetic susceptibility of rare-earth metals [3]. Recently, two systems have been identified, TmZn and TmCd, where quadrupolar pair interactions dominate and by themselves drive a phase transition [4]. The direct electric quadrupole–quadrupole interaction is small and of opposite sign to explain the experimental results obtained in refs. [1–4].

The aim of the present work is to investigate the indirect quadrupole–quadrupole interactions between rare-earth ions in metals and alloys, which arises because of the perturbation of the charge density of conduction electrons (CE) by the electric quadrupole moments of the paramagnetic ions. The influence of these indirect interactions on the ESR linewidth is studied.

(1) We use the dielectric function method [5] to calculate the induced charge density of CE due to the quadrupole moment of the paramagnetic ion at the lattice site j. Having taken into account the singularity of the dielectric function $\epsilon(\boldsymbol{k})$ at $k = 2k_F$ and the asymptotic form of the generalized function [6], having limited ourselves to terms inversely proportional to R^4, where R is the distance from the ion at the lattice site j, in the limit of large R we obtain the following expression for the induced charge density of CE:

$$\begin{aligned} n(\boldsymbol{R}) = \{ & [-F\cos(2k_F R)/R^3] \\ & + G[\ln(k_F R) + g]\sin(2k_F R)/R^4\}\Gamma_j \\ & \times (4\pi/5)^{1/2}\left\{\sum_{m=-2}^{2} Q^j_{2,m} Y^*_{2,m}(\Theta_R, \Psi_R)\right\}/6\pi, \end{aligned}$$

where

$$F = 16\pi p k_F^2/(4+pa)^2, \quad a = 1 - f(2k_F),$$
$$p = k_{FT}^2/2k_F^2, \quad G = 8\pi p^2 a k_F/(4+pa)^3,$$
$$g = \gamma - \{3(4+pa)/pa\} - 3/2, \quad \gamma = 0{,}5772.$$
$$f(k) = [(k^2/k^2 + k_F^2 + k_S^2) + (k^2/k_F^2 + k_S^2)]/4,$$
$$\Gamma = 1 - R'.$$

Here k_F is the wave vector on the Fermi surface, k_S is the inverse screening radius, $k_{FT} = (6\pi N e^2/E_F)^{1/2}$ the inverse Tomas–Fermi screening radius, N the concentration of Ce, Γ is the antishielding factor [7], Θ_R, Ψ_R are the polar angles of $\boldsymbol{R}$, and $Q_{2,m}$ is the component of the electric quadrupole moment of the paramagnetic ion.

To calculate the component $B^{ij}_{2,\xi}$ of the electric field gradient at the ion located at the lattice site i due to the induced charge density $n(\boldsymbol{R})$, the two-center integral is transformed to the one-center integral with the help of relation, proposed in ref. [8]. We suppose that the main contribution to $B^{ij}_{2,\xi}$ is due to the region with small r, where $\boldsymbol{r}$ is the radius-vector of an electron relative to the lattice site i, and restrict ourselves with contribution from the region inside the sphere with the radius $R_{ij}/2$, where $\boldsymbol{R}_{ij}$ is the radius-vector, directed from the lattice site i to the lattice site j. We limit ourselves with the terms proportional to $\ln(k_F R_{ij})/R^5_{ij}$ in calculations. The Hamiltonian of the indirect quadrupole–quadrup 'e interaction via the system of CE between the i- 1 and the j-th paramagnetic ions for a system of coordinates with the Z axis directed along the vector $\boldsymbol{R}_{ij}$ has the form [9]

$$\begin{aligned} H^{ij}_{Q-Q} &= \sum_{\xi=-2}^{2} (-1)^{\xi} B^{ij}_{2,-\xi} Q^i_{2,\xi} \\ &= \sum_{\xi=-2}^{2} (-1)^{\xi} V^{\xi}_{ij} Q^i_{2,\xi} Q^j_{2,-\xi}, \end{aligned}$$

where

$$V^{\xi}_{ij} = R^{-3}_{ij}\{F S_{\xi}(2k_F R_{ij}) + G T_{\xi}(2k_F R_{ij})\}\Gamma_i\Gamma_j,$$
$$\begin{aligned} S_0(X) = {} & (2\cos X/9) - [16\sin X\sin(X/2)/3X^2] \\ & - [(88\cos X\cos(X/2))/105X^2], \end{aligned}$$
$$\begin{aligned} S_{\pm 1}(X) = {} & (4\sin X/3X) \\ & - [(8\cos X + 32\cos X\cos(X/2))/105X^2] \\ & - [16\sin X\sin(X/2)/5X^2], \end{aligned}$$