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MAGNETIC ANISOTROPY AND MAGNETOSTRICTION OF ATOM PAIRS*

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We calculated one-electron hopping contribution to two-ion magnetic anisotropy and shape magnetostriction in amorphous $3d$-alloys. Calculations were performed in the narrow band limit and include spin–orbit coupling, the Zeeman orbital and spin magnetic moments terms with possible partial effective quenching of the orbital magnetic moments in metals. The parameters for numerical calculations are expected to correspond to pairs of Fe atoms with the spin–orbit coupling $A = 0.03$ eV and hopping integrals of about 3 eV. The magnetic anisotropy K changes its sign at some value Δ_K of effective magnetic splitting Δ proportional to the magnetization. Then the local easy axis which is parallel to the direction of the pair for small Δ switches to perpendicular easy plane case. K is nearly linear vs. Δ for small Δ and varies roughly as Δ^3 for large splitting. The dependence of magnetostriction B on Δ is similar to that of magnetic anisotropy $K(\Delta)$. For small values of Δ the coefficient B is also linear. Magnetostriction changes its sign at Δ_B and becomes positive for Δ greater than Δ_K.

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1. Introduction

The origin of magnetic anisotropy K and magnetoelastic coupling B in amorphous $3d$ alloys is of current interest. Various mechanisms may explain [1–6] experimental data on anisotropy. Also magnetostriction may be described in terms of *one-ion* or *two-ion* mechanisms. One-ion mechanism is usually understood as the interaction of asymmetric ($l > 0$) electronic clouds with neighboring atoms

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via one-electron crystal field potential. Two-ion mechanism includes all kinds of non-isotropic interactions of two magnetic atoms.

The well-established theory [7] of anisotropy and magnetostriction in insulators is not applicable [8] to $3d$ metals. Then relation between magnetic anisotropy K (or magnetostriction coefficient B) and effective magnetic splitting Δ proportional to the magnetization may be of some interest. It may help, for example, to distinguish between one-ion and two-ion mechanisms in amorphous $3d$ alloys such as FeCoNiSiB system.

The orbital magnetism and spin–orbit coupling [9–11] are considered to be a source of magnetic anisotropy and magnetoelastic coupling. In this paper we obtained numerically one-electron hopping contribution to magnetic anisotropy and shape magnetostriction of atom pairs as function of magnetic splitting Δ. Recently, this contribution was evaluated analytically in the limit of strong ferromagnetism [12] where one-electron levels were restricted to six t_{2g} states with only spin up on both atoms of the pair. Here we account for both orientations of spin. To compare these results with one-ion mechanism, we also calculated the anisotropy energy of an isolated atom with t_{2g} energy levels.

2. Method of calculations

The model Hamiltonian is

$$\mathcal{H} = A\hat{L}\cdot\hat{\sigma} - \mu_B H(2\hat{\sigma} + \alpha\hat{L}) + \sum_{\nu\nu'\sigma} t_{\nu\nu'}(a^+_{1\nu\sigma}a_{2\nu'\sigma} + \text{h.c.}) + \mathcal{H}_U - \mu\hat{N}, \quad (1)$$

where A is the one-electron spin–orbit coupling, $\hat{L}$ and $\hat{\sigma}$ are orbital and spin magnetic moments operators, ν is the orbital label and $a_{1\nu\sigma}$ ($a^+_{2\nu\sigma}$) is the annihilation (creation) operator of an electron in the state $(\nu\sigma)$. The hopping integrals $t_{\nu\nu'}$ between nearest neighbours depend on the angle of the atomic pair and on the distance between atoms, H is magnetic field and α is a phenomenological constant which measures effective partial quenching of orbital magnetic moments in metals. $\mathcal{H}_U$ is the Coulomb interaction term, μ is the chemical potential and $\hat{N}$ is the operator of the total number of electrons.

In the limit of large Coulomb repulsion U, the partition function for electrons s is

$$Z = 1 + e^{\beta\mu}\sum_{\rho}\exp(-\beta E_\rho) + e^{2\beta\mu}\left(\sum_{\tau}\exp(-\beta E_\tau)\right)^2 + O\left(\exp(-\beta U)\right), \quad (2)$$

where ρ counts one-electron states at a pair of atoms and τ labels one-electron configurations at an isolated atom. For the t_{2g} states, we adopt formulae (2) as a useful approximation valid for small average number of electrons.

We assume macroscopically isotropic system, with randomly distributed directions of atom pairs. Then shape magnetostriction is determined by a single coefficient B of the strain-dependent part of Hamiltonian,

$$B = -\partial/\partial\varepsilon\,(\partial/\partial\beta\,\ln Z), \quad (3)$$

where $\beta = 1/kT$. The derivatives are calculated for $\varepsilon = 0$. We consider the dependence of hopping elements t on the distance between atom pairs as a source of

this strain dependence. The microscopic anisotropy energy in 0 K is obtained as the difference of one-electron ground state energies of an isolated pair parallel and perpendicular to magnetization.

Parameters for numerical calculations are expected to correspond to pairs of Fe atoms: $A = 0.03$ eV [13] and hopping integrals about 3 eV [14]. Value $\alpha = 0.05$ is used since orbital admixture may be estimated from 5 to 10 per cent of spin magnetic moment. We assume small number of electrons, $n = 1$, in the sixfold degenerate t_{2g} states including spin degeneracy. The Coulomb term is accounted for as the effective field $H \equiv \Delta$ in the Hartree–Fock approximation, the results are discussed for different Δ from 0 to 1.5 eV. The one-ion anisotropy was obtained for an isolated atom with t_{2g} orbit considered in the environment distorted by a 0.1 eV downshift of the $xyf(r)$ levels to imitate the distortion.

3. Results and discussion

Figure 1 shows the anisotropy energy of atom pairs against the magnetic splitting Δ for the ferromagnetic (lower line) and antiferromagnetic (upper line) coupling. For the ferromagnetic case the energy of magnetic anisotropy changes its sign at some value of effective splitting Δ proportional to the magnetic field. For small fields, local easy axis of pair of atoms is parallel to the direction of the pair. For larger Δ, the direction of the local easy axis becomes perpendicular to the direction of the pair. This result was also obtained from our earlier analytical calculations for saturated case of large Δ. The negative anisotropy energy K varies nearly linearly as $\Delta^{0.95}$ for small values of Δ. For antiferromagnetic case, $K \sim \Delta^2$

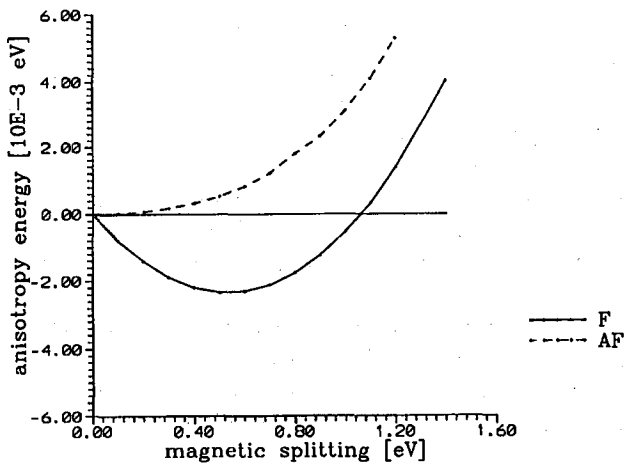

Fig. 1. Magnetic anisotropy energy of atom pair. Negative K corresponds to the easy axis along the pair.

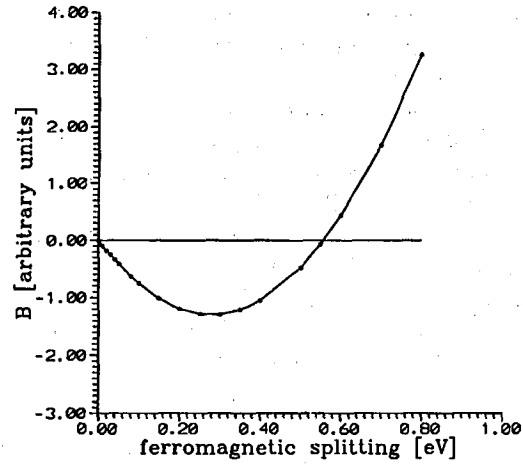

Fig. 2. Shape magnetostriction coefficient B of the system of isotropically distributed pairs of magnetic atoms against ferromagnetic splitting of energy levels.

and the local easy axis is always perpendicular to the direction of atom pair. In both cases K varies roughly as Δ^3 in the limit of large splitting. (For comparison, in the one-ion model we find similar change of sign of magnetic anisotropy, yet for small Δ this one-ion anisotropy varies as $\Delta^{1.6}$.)

We observe that the dependence of the magnetoelastic coupling B on the ferromagnetic splitting Δ is of similar nature as $K(\Delta)$ dependence, see Fig. 2. Again, for small values of the parameter Δ, the negative coefficient B is roughly linear with Δ. For larger Δ, magnetostriction coefficient changes its sign and becomes positive.

4. Conclusions

It is difficult to compare the two-ion and one-ion models. Unlike in the Callen theory for insulators, in metallic systems the two models predict similar behaviour for large Δ. For small effective splitting, exponents δ in the power law $K \sim \Delta^\delta$ are somewhat different, yet measurements of anisotropy and shape magnetostriction are most difficult in this region and so we cannot experimentally determine δ with required accuracy. However, this order-of-magnitude calculations indicate that both one- and two-ion mechanisms may significantly contribute to anisotropy and magnetostriction in $3d$ metal alloys.

Our calculations performed for isotropic system show clearly correlation between local magnetic anisotropy and macroscopic shape magnetostriction. The experimentally observed change of sign of both with increasing Δ (magnetization) was recovered in the model and it seems to be a common fingerprint of orbital magnetism.

In our calculations we assumed isotropic distribution of atom pairs. For samples with partial ordering of pairs, such as Pt_3Fe crystalline samples with ordered Fe–Fe pairs [15], it may be particularly important to calculate influence of such ordering.

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