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Fully relativistic spin-polarized description of interface exchange coupling for Fe multilayers in Au(100)

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Abstract

Magnetic anisotropy energies for two single (double) layers of Fe separated by a Au spacer and embedded in an fcc (100) Au host are calculated and discussed in terms of differences of layer-resolved total energies corresponding to different orientations of the magnetization in the Fe layers.

Consider a two-dimensional translational invariant system consisting of two multilayers of n layers of Fe, separated by an fcc(100) spacer of m layers of Au, embedded in an fcc(100) Au host (self-consistently relaxed via two additional layers of Au at the bulk interface). As is well-known, in principle the orientation of the magnetization in the Fe multilayers with respect to each other is not necessarily restricted to parallel ('ferromagnetic') and antiparallel ('antiferromagnetic') configurations. If $\boldsymbol{R}$ denotes a rotation of the orientation of the magnetization with respect to the corresponding other magnetic multilayer ($\boldsymbol{R} = \boldsymbol{E}$), then this situation can be described exactly within the so-called *fully relativistic spin-polarized Screened KKR Method* [1] such as shown in Fig. 1, where of course also the Au layers can carry induced magnetic moments. Since within this method layer-resolved quantities such as layer-resolved magnetic moments, but also layer-resolved total energies can be determined, these quantities can be investigated for different relative orientations of the magnetic field [2]. In addition such an approach offers the possibility to go beyond the so-called force theorem for anisotropy energies and allows also to perform correct layer-diagonal averaging in the case of an application of the (inhomogeneous) Coherent Potential approximation for disordered magnetic multilayers or disordered spacers.

Let $\Delta\epsilon_i(\boldsymbol{R})$ denote the following differences of layer-resolved total energies for a given arrangement of n layers of Fe and m layers of the spacer:

$$\Delta\epsilon_i(\boldsymbol{R}) = \epsilon_i(\boldsymbol{E};\boldsymbol{R}) - \epsilon_i(\boldsymbol{E};\boldsymbol{E}), \qquad (1)$$

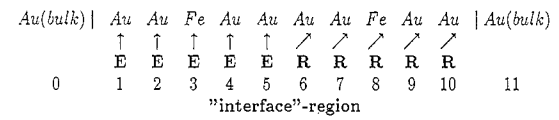

Fig. 1. Illustration of a typical interface region for Fe multilayers in Au (100).

where i specifies the layer in the 'interface' region, see above, and $(\boldsymbol{E};\boldsymbol{E})$ refers to the 'ferromagnetic' configuration. The totaldifference in energy,

$$\Delta\epsilon(\boldsymbol{R}) = \sum_{i=1}^{I} \Delta\epsilon_i(\boldsymbol{R}), \quad I = 2n + m + 4, \qquad (2)$$

can then be analyzed in terms of these layer-resolved differences. Following for example $\Delta\epsilon(\boldsymbol{R})$ as a function of $\boldsymbol{R}$ in two different systems, one obtains the situation shown in Fig. 2. One can see that for the case of the two single layers of Fe separated by six layers of Au the

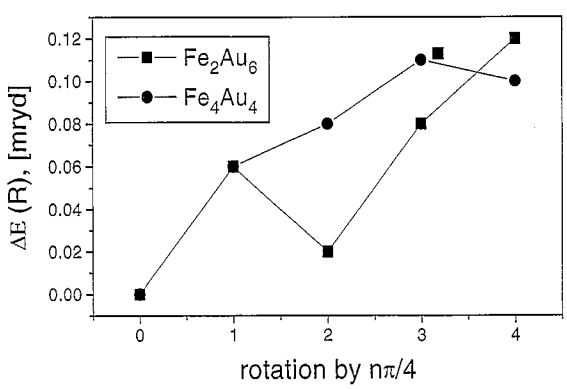

Fig. 2. Rotational dependence of the anisotropy energy for $n = 1$, $m = 6$ (Fe_2Au_6) and $n = 2$, $m = 4$ (Fe_4Au_4).

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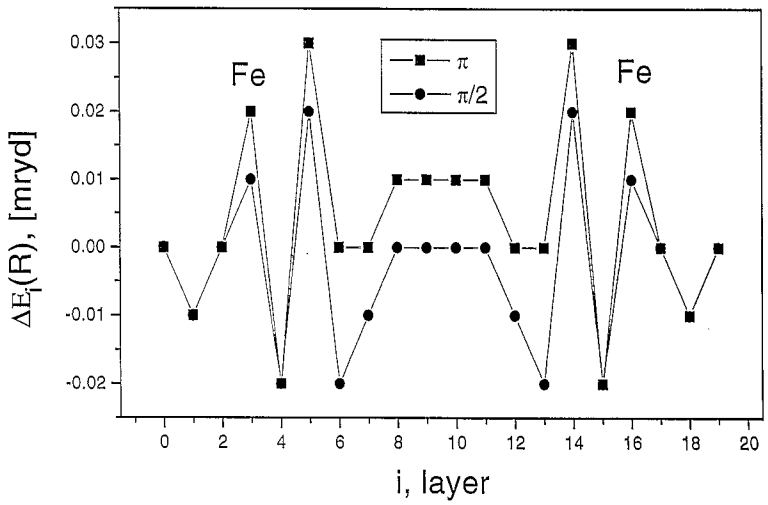

Fig. 3. $\Delta\epsilon_i(\boldsymbol{R})$ for $n = 1$, $m = 12$ (Fe_2Au_{12}). The layers indices $i = 0$ and $i = 19$ refer to the first Au bulk layers.

perpendicular orientation, $(\boldsymbol{E}; \pi/2)$, is almost as favourable as the ferromagnetic orientation. It is in particular illustrative to analyze anisotropy energies in terms of plots of $\Delta\epsilon_i(\boldsymbol{R})$ and $\Delta m_i(\boldsymbol{R})$ [2], the corresponding layer-resolved changes for the magnetic moments, with respect to layers. A very typical example for such a behaviour is shown in Fig. 3 for $\Delta\epsilon_i(\boldsymbol{R})$ in the case of two monolayers of Fe separated by 12 layers of Au. In particular Fig. 3 not only gives a very clear account of the 'local' contributions to the anisotropy energy at an Fe/Au interface, but can also serve as a physical illustration of an interface.

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References

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[2] B. Újfalussy, L. Szunyogh and P. Weinberger, Phys. Rev. B (1995), to be submitted.