Spin-orbit coupling effects on electrons, crystal field effects and magnetic anisotropy and the effect on the properties of magnetic materials

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At a fundamental level, quantum mechanical 'exchange interactions' between electrons are those interactions responsible for magnetism in condensed matter. They are, however, independent of the direction of magnetisation relative to the structural arrangement of the nuclei comprising a material. In reality, of course, the magnetisation of, say, a crystal of a magnetic material always has a preferred or 'easy' orientation and so a mechanism is required which links the spin of an electron to a spatial direction. This is provided by consideration of the relativistic effects on the motion of the electrons of which the most important and relevant is spin-orbit coupling. These relativistic interactions, which arise from the high speeds of the electrons close to the atomic nuclei and are pronounced in materials with constituents with large atomic number, are small in comparison with the exchange interactions but are nonetheless important in determining the equilibrium direction of the magnetisation, domain wall structure and magnetic properties in general [1,2].

In principle therefore, the relativistic generalisation of electronic density functional theory [3,4] (R-DFT) should provide the means to describe a magnetic material ab-initio and enable its free energy, F to be calculated. On more general micromagnetic grounds a phenomenological form of the free energy is usually written in terms of the magnetisation, $\mathbf{M}(\mathbf{r})$. A ferromagnetic material is characterised by the magnetisation in terms of M_s, the saturation magnetisation and a direction $\mathbf{n} = (\alpha_x, \alpha_y, \alpha_z)$ which is assumed to vary over length scales long compared with atomic ones, i.e. $\mathbf{M}(\mathbf{r}) = M_s \mathbf{n}(\mathbf{r})$. F is typically given as the sum of terms

$$
\begin{aligned}
F[\mathbf{M}(\mathbf{r})] \;=\; & A \int ((\nabla \alpha_x)^2 + (\nabla \alpha_y)^2 + (\nabla \alpha_z)^2) d\mathbf{r} + \int U_{an}(\alpha_x, \alpha_y, \alpha_z) d\mathbf{r} \\
& - \int \mathbf{H}^{app.}(\mathbf{r}) \cdot \mathbf{M}(\mathbf{r}) d\mathbf{r} - \frac{1}{2} \int \mathbf{H}'(\mathbf{r}) \cdot \mathbf{M}(\mathbf{r}) d\mathbf{r}
\end{aligned}
\tag{1}
$$

i.e. an exchange term with exchange constant A, an anisotropy term where $U_{an} = -K\alpha_z^2$ for uniaxial anisotropy and

$$
U_{an} = K(\alpha_x^2 \alpha_y^2 + \alpha_y^2 \alpha_z^2 + \alpha_z^2 \alpha_x^2)
\tag{2}
$$

for a cubic material (K are magnetocrystalline anisotropy constants), a term describing the interaction with an applied magnetic field and finally a magnetostatic interaction term where $\mathbf{H}'(\mathbf{r})$ is the demagnetising field due to magnetostatic volume and surface charges [2,5,6,7]. Materials are typically characterised by a set of M_s, A and K constants combined into two important length quantities, an 'exchange length', $l_{ex} = \sqrt{(A/M_s^2)}$ and a domain wall thickness $l_w = \sqrt{(A/2K)}$. R-DFT and its electronic structure basis enables M_s, A

and K to be calculated and their structural, compositional and temperature dependence found.

In the lecture the spin-orbit coupling influence on the electronic structure of materials will be described within density functional theory and its role in the origin of magnetic anisotropy, K, will be discussed in particular. The extent to which 'first-principles' R-DFT work can describe trends in K for a range of transition metal magnetic materials [4,8,9] will be reviewed. The temperature dependence of the anisotropy will be covered briefly in the context of simple spin models and then in terms of DFT models that include the effects of thermally induced 'local moment' fluctuations [10]. The effects of spin-orbit coupling upon the exchange interactions within small clusters of magnetic atoms deposited on substrates or between magnetic impurities embedded in a non-magnetic host will be described next [11]. This will enable the RKKY interaction to be revisited and pseudo-dipolar and Dzyaloshinskii-Moriya anisotropic interactions illustrated.

In transition metal systems the orbital component of the magnetisation is usually quenched by crystal field effects. In magnetic materials with 4f rare earth elements the situation is rather different. The strongly correlated f-electrons form a non-spherically symmetric charge and magnetisation density which interacts with the surrounding charge distribution. In the lecture it will be discussed how this crystal field effect and strong spin-orbit coupling leads to significant magnetic anisotropy in rare earth - transition metal magnets [1,2,9].

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