DIPOLE-DIPOLE ENERGY IN FERROMAGNETIC CRYSTALS

D.B. LITVIN

Department of Physics, University of British Columbia, Vancouver, Canada

Received 23 May 1973

The magnetic dipole-dipole energy of an array of ferromagnetic localized magnetic moments in a crystal is shown to be zero when the atom arrangement of the magnetic atoms is of cubic space group symmetry.

In the RA_{l2} (R = rare earth) intermetallic compounds, the magnetic dipole-dipole contribution to the magnetic anisotropy energy has been calculated and found to be zero [1]. The rare earth magnetic moments in these compounds are ferromagnetically aligned and the rare earth atom arrangement consists of two interlocking face-centered cubic lattices, i.e. there are two atoms per unit cell. Kittel [2] has shown the vanishing of the dipolar anisotropy energy only in the case of a ferromagnetic array of magnetic moments whose atom arrangement consists of a single cubic lattice, i.e. with only one atom per unit cell. We show below, for an arbitrary number of atoms per unit cell, that the dipole-dipole contribution to the magnetic anisotropy energy of a ferromagnetically aligned array of magnetic moments on an atom arrangement of cubic space group symmetry is necessarily zero.

The magnetic dipole-dipole energy per unit cell in a crystal with ferromagnetically aligned magnetic moments can be written as

$$E_{\text{dipole}} = \boldsymbol{S}\cdot\sum_{\boldsymbol{r}_i} \boldsymbol{E}(\boldsymbol{r}_i) \tag{1}$$

where $\boldsymbol{S}$ is the localized magnetic moment of a magnetic moment of a magnetic atom and the sum in over the positions $\boldsymbol{r}_i$ of all magnetic atoms in the unit cell. The dipolar field at $\boldsymbol{r}_i$ due to a ferromagnetic array of magnetic moments at positions $\boldsymbol{r}'$ is given by:

$$\boldsymbol{E}(\boldsymbol{r}_i) = -\sum_{\boldsymbol{r}'}^{\boldsymbol{r}_i} \frac{\boldsymbol{S}}{|\boldsymbol{r}_i-\boldsymbol{r}'|^3} + 3\sum_{\boldsymbol{r}'}^{\boldsymbol{r}_i} \frac{(\boldsymbol{r}_i-\boldsymbol{r}')[(\boldsymbol{r}_i-\boldsymbol{r}')\cdot\boldsymbol{S}]}{|\boldsymbol{r}_i-\boldsymbol{r}'|^5} \tag{2}$$

where $\boldsymbol{r}_i$ above the summation sign denotes that the sum is over all values of $\boldsymbol{r}'$ except $\boldsymbol{r}' = \boldsymbol{r}_i$.

Let $(R|\boldsymbol{\tau}(R) + \boldsymbol{t})$ denote an element of F, the space group of the magnetic atom arrangement. R is a rotation matrix, $\boldsymbol{\tau}(R)$ the non-primitive translation associated with R, and $\boldsymbol{t}$ a primitive translation. Using (2) we can write:

$$\boldsymbol{E}(R\boldsymbol{r}_i + \boldsymbol{\tau}(R)) = -\sum_{\boldsymbol{r}'}^{R\boldsymbol{r}_i+\boldsymbol{\tau}(R)} \frac{\boldsymbol{S}}{|R\boldsymbol{r}_i+\boldsymbol{\tau}(R)-\boldsymbol{r}'|^3} \tag{3}$$

$$+3\sum_{\boldsymbol{r}'}^{R\boldsymbol{r}_i+\boldsymbol{\tau}(R)} \frac{(R\boldsymbol{r}_i+\boldsymbol{\tau}(R)-\boldsymbol{r}')[(R\boldsymbol{r}_i+\boldsymbol{\tau}(R)-\boldsymbol{r}')\cdot\boldsymbol{S}]}{|R\boldsymbol{r}_i+\boldsymbol{\tau}(R)-\boldsymbol{r}'|^5}$$

Since $(R|\boldsymbol{\tau}(R))$ is an element of F we can change the summations on the right hand side of eq. (3) from over $\boldsymbol{r}'$ to over $\boldsymbol{r}'' = (R|\boldsymbol{\tau}(R))^{-1}\,\boldsymbol{r}'$. Noting that $|R(\boldsymbol{r}_i-\boldsymbol{r}'')| = |\boldsymbol{r}_i-\boldsymbol{r}''|$ and summing both sides of (3) over all elements R of the point group of F, we have that the k th component of the resulting sum is

$$\sum_R \boldsymbol{E}_k(R\boldsymbol{r}_i+\boldsymbol{\tau}(R)) = -N\sum_{\boldsymbol{r}''}^{\boldsymbol{r}_i} \frac{\boldsymbol{S}_k}{|\boldsymbol{r}_i-\boldsymbol{r}''|^3} \tag{4}$$

$$+3\sum_{\boldsymbol{r}'',m,n,l}^{\boldsymbol{r}_i} \frac{(\boldsymbol{r}_i-\boldsymbol{r}'')_m(\boldsymbol{r}_i-\boldsymbol{r}'')_l\boldsymbol{S}_n}{|\boldsymbol{r}_i-\boldsymbol{r}''|^5} \sum_R R_{km}R_{nl}$$

where N is the order of the point group of F.

If F is a cubic space group, i.e. with point group T, T_h, O, T_d, or O_h, the matrices R constitute a real three dimensional irreducible representation of the point group. One can then perform the summation over R on the right-hand side of (4) using the orthogonality relation [3] $\Sigma_R R_{km}R_{nl} = \frac{1}{3}N\delta_{kn}\delta_{ml}$. Doing this and then summing over m, n, and l one derives:

$$\sum_R \boldsymbol{E}(R\boldsymbol{r}_i+\boldsymbol{\tau}(R)) = 0. \tag{5}$$

Since $\boldsymbol{r}_i, R_2\boldsymbol{r}_i+\boldsymbol{\tau}(R_2), \ldots, R_N\boldsymbol{r}_i+\boldsymbol{\tau}(R_N)$ constitute a set of equivalent positions in the unit cell of F, (5)

is interpreted as follows: The vector sum of the dipole fields, due to a ferromagnetic array of magnetic moments whose magnetic atom arrangement is of cubic symmetry F, on a set of equivalent positions in the unit cell of F is zero. Since the sum over $\boldsymbol{r}_i$ in (1) can be subdivided into sums over sets of equivalent positions in the unit cell, we have that when F is a cubic space group, as in the rare earth intermetallic compounds, the magnetic dipole-dipole energy vanishes.

The author would like to express his thanks to N. Kaplan for pointing out this problem.

References

[1] N. Kaplan, E. Dormann, K.H.J. Buschow and D. Lebenbaum, Phys. Rev. 7 (1973) 40.
[2] C. Kittel, Rev. Mod. Phys. 21 (1949) 541.
[4] M. Hamermesh, Group theory (Addison-Wesley Publishing Co., Reading, Mass., 1962) p. 103.