DIPOLE MAGNETIC ANISOTROPY FIELDS IN RHOMBOHEDRAL ANTIFERROMAGNETIC MATERIALS

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Results of calculations of the contribution of magnetic dipole interactions to the effective uniaxial anisotropy fields of antiferro- and ferromagnetism vectors in rhombohedral antiferromagnetic materials with the S ions are given as functions of the ratio of the hexagonal crystal cell parameters $c_H/a_H$. There is a strong dependence of the calculated curves on the lattice parameters of real compounds. From the dependences obtained the effective anisotropy fields are calculated for FeF$_3$, FeBO$_3$, and MnCO$_3$.

The problem of calculating the dipole crystalline interaction energy is associated not only with the conditional convergence of the lattice sums that, however, can be transformed into absolutely fast-converging series using the existing methods [1, 2] but also with their cumbersome expressions. Long expressions for these series may readily result in calculation errors. Therefore, to obtain objective information on dipole crystalline field magnitudes, their dependences on the crystal-lattice parameters are constructed, from which conclusions are drawn regarding the reliability of the quantities being calculated.

The thermodynamic potential, considering the second-order uniaxial anisotropy invariants of antiferro- and ferromagnetism vectors in crystals of the spatial symmetry group $D_3h$, has the form [3]

$$\Phi = (a_M) l^2 + (b_M) m^2,$$

where $l = M_1 - M_2$ and $m = M_1 + M_2$ are the antiferro- and ferromagnetism vectors and $M_1$ and $M_2$ are the magnetic sublattice moments per mole of the substance.

Changes in the thermodynamic potential corresponding to transitions of the vectors $l$ and $m$ from states $(1) l = M$, $m = 0$ and $(2) m = M$, $l = 0$ to states $(3) l = 0$, $m = 0$ and $(4) m = 0$, $l = 0$, respectively, have the forms

$$\Phi(1) - \Phi(3) = aM^2/2, \quad \Phi(2) - \Phi(4) = bM^2/2,$$

where $M = 2 |M_1| = 2 |M_2|$. Equating Eqs. (1) to the corresponding changes in the dipole crystalline energies $E(1) - E(3)$ and $E(2) - E(4)$, we will obtain

$$a_{\text{dip}}M^2 = 2[E(1) - E(3)],$$

$$b_{\text{dip}}M^2 = 2[E(2) - E(4)].$$

We will calculate the energies $E(i)$ ($i = 1, 2, ..., 4$) for the hexagonal cell. The ion coordinates $j_1$, $j_2$, and $j_3$ are given in Table 1.

The dipole energy of the crystal in state $i$ can be represented in the form

$$E(i) = (1/2) \sum_{k,l} e_{kl}(i),$$

where $e_{kl}(i)$ is the energy of the interaction between the $k$th dipole and the dipoles of the $l$th sublattice per mole of the
TABLE I

<table>
<thead>
<tr>
<th>k, l</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
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<td>1/3</td>
</tr>
<tr>
<td>j_3</td>
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<td>1/2</td>
<td>1/3</td>
<td>1/6</td>
<td>2/3</td>
<td>5/6</td>
</tr>
</tbody>
</table>

substance (altogether there are 6 sublattices constructed from the primitive hexagonal cells, according to the number of ions in the elementary cell).

The dipole energy $\varepsilon_{kl}(i)$ for $i = 1, 2, \ldots, 4$ will assume the form

$$\varepsilon_{kl}(1,2) = \left(\frac{N}{6}\right) m_{kl} m_{ll} \sum_{\alpha_{kl}} \left[ \frac{1}{r_{2\alpha_{kl}}} \left[ 1 - 3 \frac{z^2_{\alpha_{kl}}}{r^2_{\alpha_{kl}}} \right] \right],$$

$$\varepsilon_{kl}(3,4) = \left(\frac{N}{6}\right) m_{kl} m_{ll} \sum_{\alpha_{kl}} \left[ \frac{1}{r_{2\alpha_{kl}}} \left[ 1 - 3 \frac{y^2_{\alpha_{kl}}}{r^2_{\alpha_{kl}}} \right] \right],$$

where $m_k$ and $m_l$ are the magnetic moments of the $k$th and $l$th dipoles of the corresponding sublattices, $r_{\alpha_{kl}} = \sqrt{x^2_{\alpha_{kl}} + y^2_{\alpha_{kl}} + z^2_{\alpha_{kl}}}$ is the distance between the interacting dipoles, and $\alpha_{kl}$ is the summation index. In the derivation of these expressions, we took into account that in the approximation being considered the dipole energy is independent of the senses of vectors $l$ and $m$ in the basal crystal plane for the spatial symmetry group $D_6^5$ [2]. The product $m_k m_l$ ($\xi = y, z$) in the state with $i = 1, 3$ will be positive or negative depending on whether the interacting dipoles belong to one or different magnetic sublattices. With this circumstance taken into account, $\varepsilon_{kl}(i)$ can be written in the form

$$\varepsilon_{kl}(i) = (-1)^{(k+i)} \left( \frac{N m_0^2}{6} \right) (-S_{kl}^\xi),$$

$$S_{kl}^\xi = \sum_{\alpha_{kl}} \left[ \frac{1}{r_{2\alpha_{kl}}} \left[ \frac{e_{\alpha_{kl}}^2}{r_{2\alpha_{kl}}} - 1 \right] \right].$$

($\xi = z$ for $i = 1, 2$ and $\xi = y$ when $i = 3, 4$), where $m_0$ is the magnitude of the ion magnetic moment. The condition of the independence of the dipole crystalline energy from the choice of the coordinate system and the equivalence of the $k$th and $l$th primitive hexagonal cells yield that in the matrix $E(i)$

$$E_{kk} = \varepsilon_{ll}, \quad \varepsilon_{kl} = \varepsilon_{lk}. \quad (4)$$

The symmetry of the crystal lattice and of the expressions leads to relations

$$\varepsilon_{13} = \varepsilon_{15} = \varepsilon_{24} = \varepsilon_{26} = \varepsilon_{35} = \varepsilon_{46},$$

$$\varepsilon_{14} = \varepsilon_{16} = \varepsilon_{23} = \varepsilon_{25} = \varepsilon_{34} = \varepsilon_{26},$$

$$\varepsilon_{12} = \varepsilon_{36} = \varepsilon_{45}. \quad (5)$$

With Eqs. (4) and (5) taken into account we will obtain

$$E(i) = \left(\sqrt{2}\right) \left[ 6 \varepsilon_{11}(i) + 12 \varepsilon_{13}(i) + 12 \varepsilon_{14}(i) + 6 \varepsilon_{12}(i) \right]. \quad (6)$$

Substituting Eq. (3) into Eq. (6) we have