2.13. Study of internal fields in $BiFeO_3$ by Mössbauer spectroscopy

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The antiferromagnetic-ferroelectric ferrite $BiFeO_3$ with weak ferromagnetic properties[1] was studied by Mössbauer efect[2] in the temperature range from 8° — 760°K. The measured spectra show bellow the Neel temperature $T_N = 643$°K six line distribution characteristic for a strong magnetic hyperfine interaction while above the Neel temperature T_N have two peaks shape typical for quadrupole interaction.

At 9°K spectrum yields the internal magnetic field of 548 ± 10 KG, isomer shift relative to metallic iron of 0.56 ± 0.05 mm/sec and quadrupole splitting of 0.42 ± 0.05 mm/s. The values above 90°K agree with the results published recently by Biran et al.[3]

The angle Θ between the electric field gradient and the direction of the internal magnetic field can be estimated on the base of Kunding[4] analysis as 80°—90°. The Morin transition induced by the turning of the electron spins over 90° has not been observed down to 8°K.

Molecular field approximation with the Brillouin function for $S = 5/2$ and $H_0 = 550$ KG fits the experimental values for relative internal magnetic fields in the range 8°K — 640°K, while the spin wave T^2 approximation is satisfying in the range bellow 260°K. Both approximations lead to the same value for the exchange integral $|J|k^{-1} = 36.7$.

With the value determined for quadrupole splitting $\Delta E = 0.38 \pm 0.04$ mm/s at 670°K and with the assumed quadrupole moment for iron in 14,4 keV state $Q = 0.41$ barn[5], the field gradient results as $V_{zz} = 9.1 \pm 0.2 \cdot 10^{17}$ V/cm^2.

Using the reported data of unit cell obtained by the electron diffraction[5] analysis the components of electric field gradient have been calculated by the point charge lattice sum with the Wette-Schacher[7] planewise method. Result is axially symmetric electric field gradient with the principle exis $V_{zz} = 4.3 \cdot 10^{16}$ V/cm^2 paralel to the threefold (111) axis. The disagreement between the calculated and the measured value could be explained by the uncertainty of the positions of ions and of the quadrupole moment and by the neglect of the covalent bonding effect at iron ion. The latest data[1,8] for the positions of ions at 600°C bring calculated value for V_{zz} closer to the measured one which indicates strong dependence of V_{zz} for changes in ion parameters in the lattice.

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