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Mössbauer study of polycrystalline multiferroic Ba-doped $BiFeO_3$ compound

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Recently, both ferroelectricity and ferromagnetism in $Bi_{0.7}Ba_{0.3}FeO_3$ compound were observed at room temperature by *P-E* and *M-H* loop measurements, respectively.[1,2] We prepared a $Bi_{0.7}Ba_{0.3}FeO_3$ sample by a rapid two-stage solid state reaction method. An analysis of x-ray diffraction pattern by Rietveld refinement method using FULLPROF program shows that the sample has a rhombohedrally distorted perovskite structure with the lattice constant a = 4.2389 Å, c = 13.4256 Å. The $Bi_{0.7}Ba_{0.3}FeO_3$ compound have two different crystal sites for iron ions, i.e. the octahedral sites and the oxygen-deficient tetrahedral sites. Mössbauer spectra of $Bi_{0.7}Ba_{0.3}FeO_3$ was obtained at various absorber temperatures from 4.2 K to the Néel temperature. The Mössbauer spectrum at 4.2 K was fitted to two magnetic components of the magnetic hyperfine fields H_{hf} = 549 kOe for octahedral sites and H_{hf} = 521 kOe for oxygen-deficient tetrahedral sites. The isomer shift value at room temperature is found to be 0.27 and 0.23 mm/s relative to the Fe metal, which is consistent with high-spin Fe^{3+} charge states. The electric quadrupole splittings (ΔE_Q) are observed with large values of 0.13 mm/s for oxygen-deficient tetrahedral sites compared to 0.03 mm/s for octahedral sites. The Néel temperature (T_N) and the Debye temperature are found to be 750 ± 5 K and 321 ± 1 K, respectively. Plots of the reduced magnetic hyperfine field $H_{hf}(T)/H_{hf}(0)$ against reduced temperature T/T_N for octahedral sites of $Bi_{0.7}Ba_{0.3}FeO_3$ sample showed Brillouin curve B(S) for S = 5/2. But it showed the deviation from the Brillouin variation for oxygen-deficient tetrahedral sites. It might be due to spatially complicated spin structure. Magnetization measurements indicate ferromagnetic behavior with hysteresis loops at room temperature. The coercivity value (H_c) is 2485 Oe. The strong coercivity force may result from the magnetic anisotropy.

[1] M. Gajek et. al., Nature Mater., 6, 296 (2007).
[2] D. H. Wang et. al., Appl. Phys. Lett., 88, 212907 (2006)