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Multiferroic Bismuth Ferrite: First PAC and XRD studies on its ferroic alpha-beta phase transition

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Work of numerous research groups has shown different outcomes of studies of the transition from the ferroelectric α-phase to the high temperature β-phase of the multiferroic, magnetoelectric perovskite Bismuth Ferrite ($BiFeO_3$ or BFO). Using the perturbed angular correlation (PAC) method with ^{111m}Cd as the probe nucleus, the α to β phase transition was characterized. These are the first data on ^{111m}Cd in BFO so far. The phase transition temperature, the change of the crystal structure and its parameters were supervised with measurements at different temperatures using a six detector PAC setup to observe the γ-γ decay of the ^{111m}Cd probe nucleus. The temperature dependence of the hyperfine parameters shows a change in coordination of the probe ion, which is substituting the bismuth site, forecasting the phase transition. A visible drop of the quadrupole frequency ω_0 at a temperature of about $T_c \approx 820°$C is indicating the α-β phase transition. Matching results with Density Functional Theory (DFT) simulations suggest orthorhombic $Pbnm$ crystal symmetry for the high temperature β-phase. This structure is proven from a nuclear point of view. Combined with high temperature x-ray diffraction (XRD) measurements also showing the beta phase appearing in $Pbnm$ setting, a general description of the β-phase could be made.

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