High-resolution Powder Diffraction Study of $BiFeO_3$ Nanoparticles

C.U. Segre,[1] S. Chattopadhyay,[1,2] V.R. Palkar[3]
[1]Biological, Chemical and Physical Sciences Department, Illinois Institute of Technology, Chicago, IL, U.S.A.
[2]Advanced Photon Source (APS), Argonne National Laboratory, Argonne, IL, U.S.A.
[3]Tata Institute of Fundamental Research, Mumbai, India

Introduction

$BiFeO_3$ is one of only a few magnetoelectric materials that exhibit both ferroelectric and magnetic ordering [1, 2]. Size effect studies of nanoparticulate $BiFeO_3$ indicate that as the particle size decreases, the Neel temperature (T_N) decreases from 400 to 339°C, and the antiferromagnetic-to-paramagnetic transition becomes increasingly diffuse [3].

Methods and Materials

We report here on the results of room-temperature powder diffraction studies of the lattice parameter and particle size of $BiFeO_3$ nanoparticles prepared by a wet-chemistry coprecipitation technique. The samples were packed in capillaries (2 mm diameter) that were rapidly rotated during the measurement in transmission mode at the MR-CAT beamline at the APS. The incident radiation was 0.4958 Å, and a Si(111) flat analyzer crystal was placed in front of the scintillation detector. Four samples of $BiFeO_3$ with varying particle sizes were measured for this report.

Results and Discussions

$BiFeO_3$ crystallizes in a hexagonal (rhombohedral) distorted perovskite structure. The (102) and (110) reflections for the two samples with the smallest and largest particle sizes are shown in Fig. 1. Note the shift in position, which indicates a small change in lattice parameters as a function of particle size. The diffraction patterns were analyzed by using a total pattern fitting program that is used for extracting lattice constants and peak widths without refining details of the crystal structure, such as atomic positions. The resulting lattice parameters, volumes, and nominal and measured particle sizes are shown in Table 1.

The measured particle size is consistent with the nominal size; however, there appears to be very little lattice expansion as a function of particle size in this range.

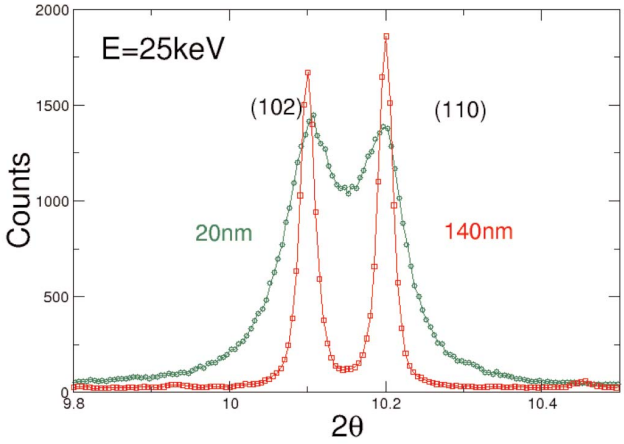

FIG. 1. Details of the (102) and (110) diffraction peaks of two $BiFeO_3$ samples, with nominal particle sizes as shown.

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TABLE 1. Nominal particle sizes, lattice constants, and measured sizes for BiFeO3 samples.

Nominal Size (nm)	a (nm)	c (nm)	V (nm^3)	Measured Size (nm)
140	0.55789 ±1	1.3869 ±2	37.38	80
44	0.55791 ±1	1.3869 ±2	37.38	65
25	0.55758 ±4	1.3850 ±1	37.29	42
20	0.55828 ±4	1.3862 ±1	37.42	24

[a]The measured particle sizes were calculated by using the Scherrer equation on the (204) reflection and LaB6 as a standard.