Crystal growth mechanism and ferroelectric domains in BiFeO₃ nanoparticles

Xiaofei Bai^{a*}, Pavan Nukala^b, Jie Wei^c, Maria Varela^d, Nicolas Guiblin^b, Brahim Dkhil^b, Ingrid Canero-Infante^a

- a. CNRS, Institut des Nanotechnologies de Lyon, CNRS UMR5270 ECL INSA UCBL CPE, 7, Avenue Jean Capelle, 69621, Villeurbanne, France
- b. Laboratoire Structures, Propriétés et Modélisation des Solides (SPMS), CentraleSupélec, CNRS-UMR8580, Université Paris-Saclay, Gif-sur-Yvette, France
- c. Electronic Materials Research Laboratory, Key Laboratory of Ministry of Education & International Center for Dielectric Research, Xi'an Jiaotong University, Xi'an 710049, People's Republic of China
- d. Departamento de Fisica de Materiales & Instituto Pluridisciplinar, Universidad Complutense de Madrid, Madrid 28040, Spain
- * xiaofeibxf@gmail.com

Abstract: BiFeO₃, as a promising multiferroic material, has attracted strong interest for acoustics, optical, electrical and magnetic study. Here we systematically designed a wetchemical synthesis process with two optimizing thermal treatment steps to obtain singlephase BiFeO₃ nanoparticles via Differential Scanning Calorimetry. The pure phase is confirmed from powder X-ray diffraction. Further, ferroelectric domains in nanoparticles are observed by high resolution transmission electron microscopy, with Fe displacements of 35 pm contributing to the polarization and ferroelectricity in our nano BiFeO₃. Through Electron Energy Loss Spectroscopy, a local octahedral ligand environment around Fe³⁺ is confirmed, which character of *R3c* in BiFeO₃ nanoparticles. Finally, we thoroughly analysed the growth kinetics via Johnson-Mehl-Avrami thermal kinetic model and deduced that the crystallization mechanism of our nano BiFeO₃ is surface nucleation from precursor powders. Our findings therefore furnish a practical method for synthesizing high quality nano BiFeO₃ and highlight the ferroelectricity in BiFeO₃ nanoparticles which rely on the interface coupling.