MS40-2-6 In situ 3D observations of a core-shell volume transition in an Ni_3Fe nanocrystal using Bragg coherent X-ray diffraction imaging
#MS40-2-6

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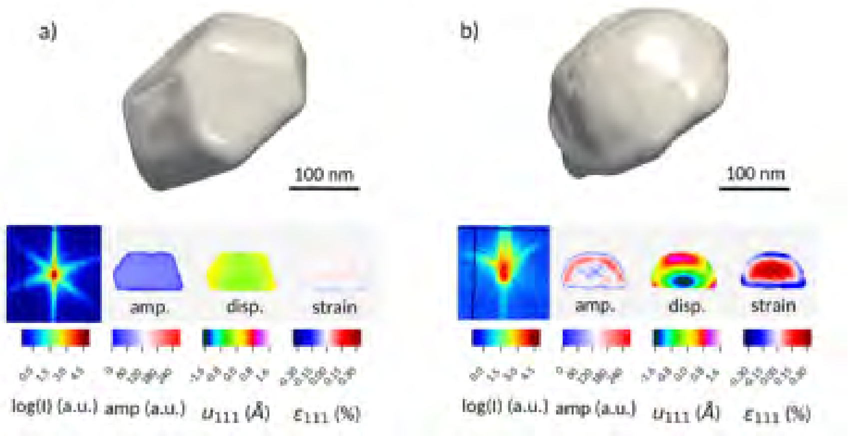
Abstract
Coherent X-ray Diffraction Imaging (CDI) [1] allows for the *in situ* 3D mapping of the structural changes during phase transitions and chemical reactions, with a fair spatial resolution of the order of magnitude of 10 nm [2]. Using this technique in multi-Bragg conditions (Bragg CDI on multiple reflections), it was possible to follow the structural evolution (change in morphology, variation of the displacement and strain fields) as a function of temperature in a 300 nm Ni_3Fe nanocrystal. During this volume transition, which happens between 500°C and 600°C, a core-shell structure is progressively observed with two distinct lattice parameters (difference of 0.39%, corresponding to two different Ni:Fe ratios), leading to highly strained and coherent domains. A rounding of the particle is also observed, with a disappearing of the initial facets. Static molecular calculations (LAMMPS) of different systems, such as faceted and core-shell nanoparticles, complete this work and allow for the confirmation of a core-shell structure. This study shows the perfect ability of modern phase retrieval methods to reconstruct highly strained systems such as core-shell nanoparticles.

References
[1] I. Robinson and R. Harder, Coherent X-Ray Diffraction Imaging of Strain at the Nanoscale, Nat. Mater. 8, 291 (2009).
[2] S. Labat, M.-I. Richard, M. Dupraz, M. Gailhanou, G. Beutier, M. Verdier, F. Mastropietro, T. W. Cornelius, T. U. Schülli, J. Eymery, and O. Thomas, Inversion Domain Boundaries in GaN Wires Revealed by Coherent Bragg Imaging, ACS Nano 9, 9210 (2015).

BCDI analysis (a) before and (b) after annealing



LAMMPS simulations: (a) faceted and (b) core-shell