Study of Y_2O_3 nanoparticles by x-ray absorption spectroscopy

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Nanocrystalline Y_2O_3 finds many applications as rare-earth doped nanophosphor, gate material in integrated circuits, an additive in many structural and functional ceramics as well as in oxide dispersion strengthened steels. Chemically pure cubic and monoclinic Y_2O_3 nanoparticles can be obtained at room temperature and atmospheric pressure [1]. Note that cubic Y_2O_3 nanoparticles are more stable than their bulk counterparts against pressure-induced amorphization [2]. Understanding of nanoparticles properties at the atomic scale represents a complicated task which should be addressed using joint effort based on modern experimental and theoretical approaches.

In this study we have used the Y K-edge extended x-ray absorption fine structure (EXAFS) spectroscopy to validate a number of theoretical force-field models [3-4] by MD-EXAFS method [5] and to check the sensitivity of the EXAFS technique to particle size.

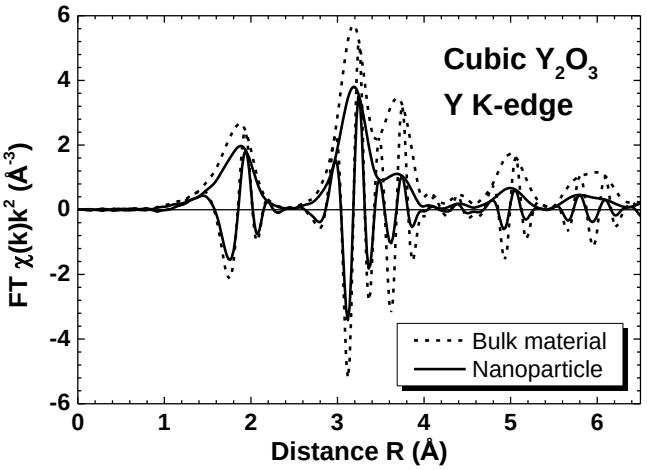

Fig. 1. Fourier transforms (modules and imaginary parts) of the calculated Y K-edge EXAFS for bulk material (dashed lines) and 1 nm nanoparticle (solid lines) cubic Y_2O_3.

Our results suggest that the force-field model developed in [4] describes in the best way the structure and lattice dynamics in cubic Y_2O_3 and allows one to reproduce the behaviour of the temperature-dependent Y K-edge EXAFS spectra in the range of 300-1273 K. Our simulations also show strong sensitivity of the EXAFS technique to Y_2O_3 nanoparticle size, which is clearly observed (Fig. 1) as a significant reduction of the outer shell contributions due to surface effect.

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