Static disorder in nanocrystalline yttria probed by X-ray absorption spectroscopy

Inga Jonane, Janis Timoshenko, Alexei Kuzmin
Institute of Solid State Physics, University of Latvia, Latvia
e-mail: ingajonaane@gmail.com

Yttria (Y_2O_3) is an important material for technological applications. During the last decade Y_2O_3 attracted much attention since it was shown that mechanical properties and radiation resistance of steels can be improved by formation of nanosized yttria within the steel matrix [1]. Such steels are considered now as promising structural materials for concentrated solar power plants and jet engines, and, in particular, for fusion and fission nuclear reactors.

The understanding and improving of properties of nanosized particles at atomic scale represents a complicated task which should be addressed using modern experimental and theoretical approaches. In this study we have investigated the local structure of crystalline and nanocrystalline Y_2O_3 using the Y K-edge X-ray absorption spectroscopy. The extended X-ray absorption fine structure (EXAFS) has been interpreted using the recently developed reverse Monte Carlo and evolutionary algorithm (RMC/EA) approach [2] (Fig.1). This approach allowed us to compare local structures of nanosized and crystalline yttria and to estimate the effects of structural and thermal disorder.

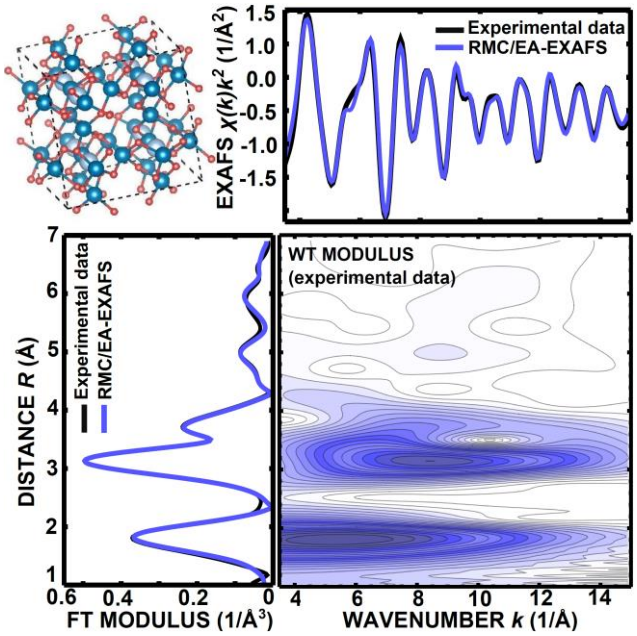

Fig.1 Results of RMC/EA EXAFS calculations for nanocrystalline Y_2O_3: experimental and simulated Y K-edge EXAFS spectra (upper panel), their Fourier transforms (FT, left panel) and the wavelet transform (WT) of experimental data (bottom right panel).

Participation is supported by ERAF project No. 2015/0014/2DP/2.1.1.2.0/14/APIA/VIAA/010

References

1. S. Ukai, M. Fujiwara, J. Nucl. Mater. **307,** 749 (2002)
2. J. Timoshenko, A. Kuzmin, J. Purans, J. Phys.: Condens. Matter. **26**, 055401 (2014).