Poster Presentation

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Simulation based approach to structure relaxation in oxides nanomaterials

A. Kuzmin[1], A. Anspoks[1], A. Kalinko[2], J. Timoshenko[1]

[1]University of Latvia, Institute of Solid State Physics, Riga, Latvia, [2]Synchrotron SOLEIL, l'Orme des Merisiers, Saint-Aubin, France

Physical properties of nanoparticles depend strongly on their structure, therefore an understanding of atomic structure relaxation at nanoscale is very important for properties tuning but is a challenging task. Upon crystallite size reduction below about 10 nm, the unit-cell volume expansion is observed in most nanooxides, opposite to metal nanoparticles. The detailed understanding of this phenomenon requires joint use of modern experimental and theoretical methods. In this study we will illustrate how the nanostructure problem can be addressed using classical molecular dynamics [1] and reverse Monte Carlo [2] simulation methods, employed to the analysis of synchrotron radiation x-ray absorption spectra. The two simulation based approaches allow us to obtain structural models which account for the nanoparticle size, thermal disorder and high-order correlation effects. Two examples of their use will be discussed in details: (i) the role of nickel vacancies in nickel oxide nanoparticles/thin films and (ii) the effect of transition metal type on tungstate nanoparticles.

[1] *A. Anspoks, A. Kalinko, R. Kalendarev, et al, Phys. Rev. B, 2012, 86, 174114:1-11.,* ***[2]*** *J. Timoshenko, A. Kuzmin, J. Purans, J. Phys.: Condens. Matter, 2014, 26, 055401:1-15.*

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