Institute of Solid State Physics, University of Latvia
Material Science for Fusion and Fission

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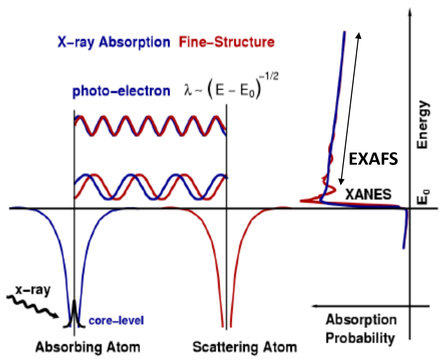
The Institute of Solid State Physics, University of Latvia (ISSP UL), is the leading research centre in Latvia that can provide internationally comparable research in materials science, educate students in modern technology and material studies, and provide innovative solutions for industrial applications (Technopolis group research assessment, 2013). Its international competence was acknowledged already in 2001 when the Institute received the "Excellence Centre of Advanced Materials Research and Technology" award by the European Commission.

ISSP UL can apply presented knowledge gained in EUROfusion and EURATOM projects to other projects in fusion and fission sector

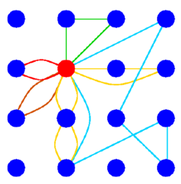
X-ray Absorption Spectroscopy

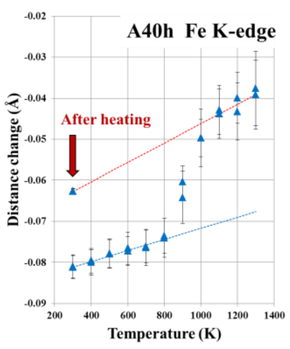


X-ray Absorption Spectroscopy (**XANES/EXAFS**) probes local atomic and electronic structure as well as lattice dynamics.

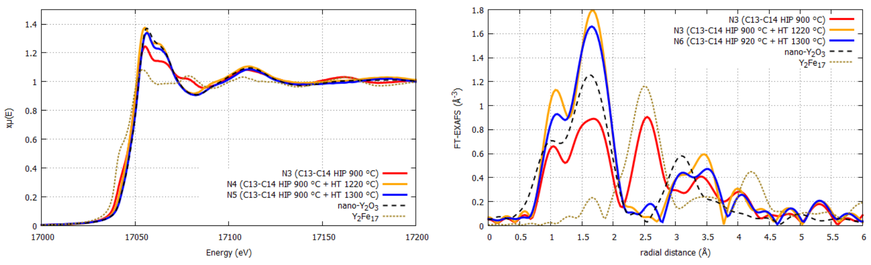
$$\chi_n^l(k) = \sum_i A_n^l(k,R_i)\sin(2kR_i + \Psi_n^l(k,R_i))\exp(-2\sigma_i^2 k^2)$$

$$\chi_2^l(k) = \int_{R_{\min}}^{R_{\max}} \frac{G(R)}{kR^2} F(k,R)\sin(2kR + \Psi(k,R))dR$$





In situ heating of Austenitic ODS steel

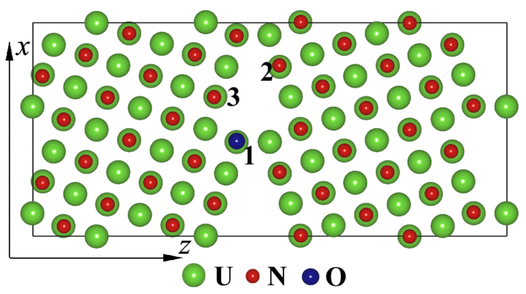


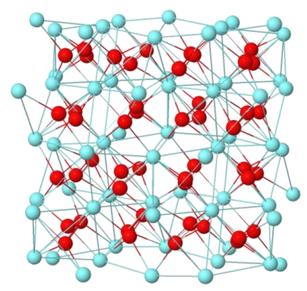
Y K-edge XANES (on the left) and FT-EXAFS (on the right) for ODS samples HIP 900°C (red), after heat treatment 1220°C (orange), 1300°C (blue), and nano-Y_2O_3 (black dash), Y_2Fe_{17} (olive dotted) reference samples.

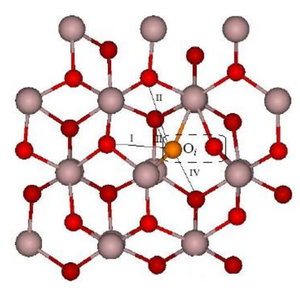
Theoretical Physics and Computer Modelling Dept

Main research activities: large scale, massive parallel**, first principles calculations** of the atomic and electronic structure and **Kinetic Monte Carlo** modeling of advanced materials for both fusion and fission applications. Real experience in the field is gained in:

- modeling of new nuclear fuels (e.g. UN and its oxidation),
- formation process of yttria nanoclusters in ODS steel for fusion ,
- study of radiation stability and material damage in reactor functional materials (e.g. Al_2O_3 and other oxides used for optical windows etc.)







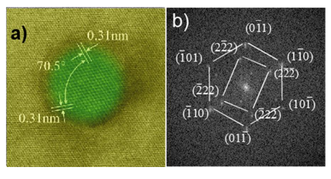
Combining Experiment and Theory

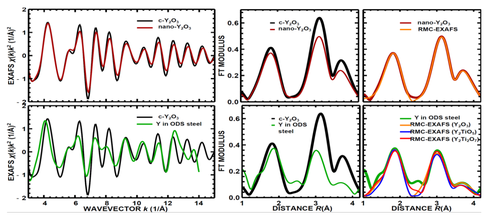
EUROfusion Enabling Research project "When and how ODS particles are formed?" combines X-ray Absorption Spectroscopy and theoretical modelling.

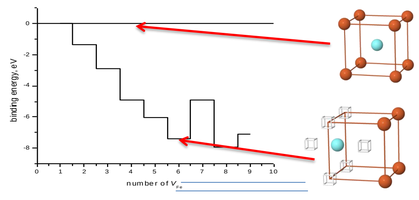
Experimental part contains preparation of the model materials and state-of-the-art in operandi experiments using synchrotron radiation to study behaviour of Y and Ti atoms in the Fe, Fe/Cr, and ferritic steel matrix, from metallic state to disperse oxide nanoparticles.

The first step of theoretical modelling includes *ab initio* calculations on the interaction between impurity atoms and Fe vacancies. It is clearly shown that oxygen atoms or O atoms with Fe vacancies are required to form inter-atomic binding in Y_2O_3 nanoclusters. We also calculated migration barriers of impurity atoms and clusters of vacancies. The second step includes simulation of precipitate growth based on results of *ab initio* calculations and employs the lattice kinetic Monte Carlo (LKMC) simulations on the matrix and interstitial sublattices.

Project includes also theoretical model validation as final stage.



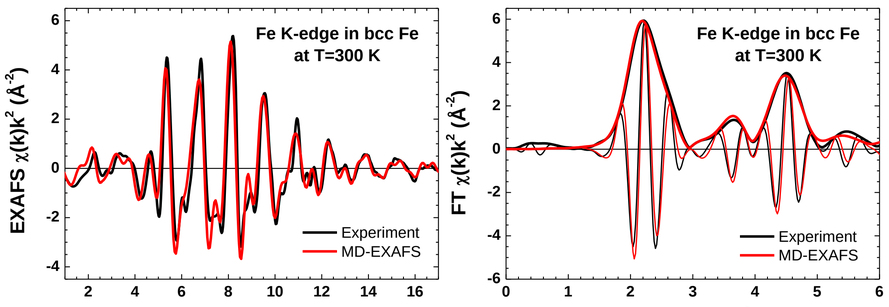




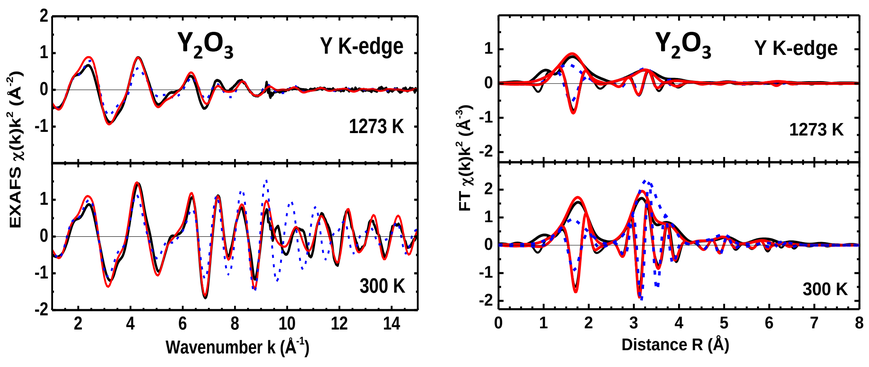
EXAFS as model validation tool

We demonstrate the use of the extended x-ray absorption fine structure (EXAFS) for the validation of the force field models based on the approach developed in [1-3]. The EXAFS spectrum can be relatively easy measured (also at extreme conditions) for bulk and nanocrystalline materials and can be directly compared with the configuration-averaged EXAFS, obtained using the results of the molecular dynamics (MD) simulation, to conclude on the force field model reliability [1,3]. The application of the method to several materials including bcc Fe, Y_2O_3, Y_2TiO_5 and $Y_2Ti_2O_7$, UO_2 is given below.

[1] A. Kuzmin and R.A. Evarestov, J. Phys.: Condens. Matter 21 (2009) 055401 (6 pp).
[2] A. Kuzmin and J. Chaboy, IUCrJ 1 (2014) 571-589.
[3] A. Kuzmin, A. Anspoks, A. Kalinko, J. Timoshenko, Z. Phys. Chem. 230 (2016) 537-549.



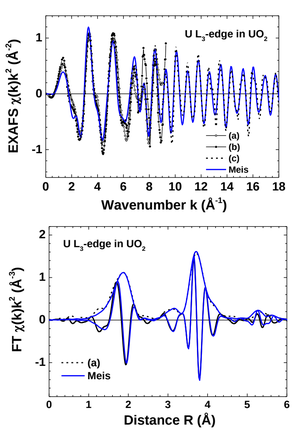
Validation of Embedded Atom Model (EAM) force field model for **Fe** from M.W. Finnis and J.E. Sinclair, Phil. Mag. A 50 (1984) 45.



Model 1: P. P. Bose, M. K. Gupta, R. Mittal, S. Rols, S. N. Achary, A. K. Tyagi, S. L. Chaplot, Phys. Rev. B 84 (2011) 094301.

Model 2: K. C. Lau, B. I. Dunlap, J. Phys. Condens. Matter 23 (2011) 035401.

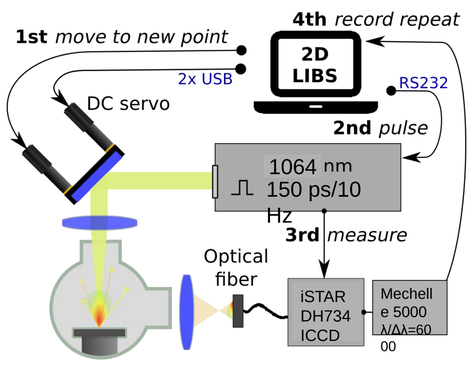
Comparison between the experimental (solid lines) and MD-EXAFS calculated, dashed lines: Model 1; dotted lines: Model 2, Y K-edge EXAFS spectra $\chi(k)k^2$ and their (phase-uncorrected) Fourier transforms for c-Y_2O_3 at 300 and 1273 K.

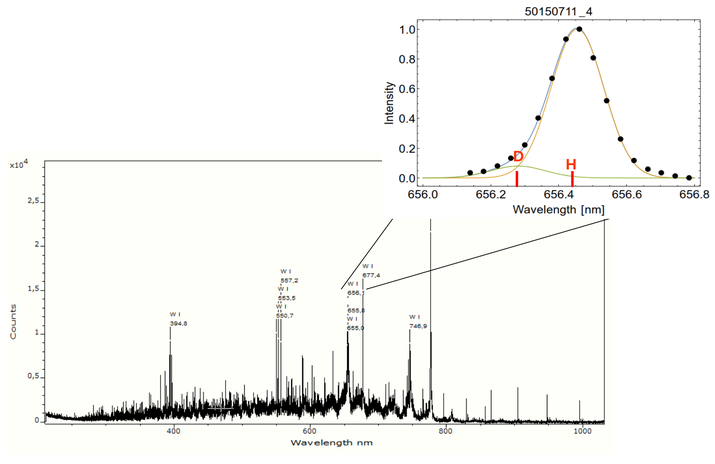


Comparison of the experimental and calculated U L_3-edge EXAFS $\chi(k)k^2$ and their Fourier transforms (FTs) for UO_2 at T = 300 K. The experimental EXAFS signals correspond to (a) UO_2, (b) irradiated Cr-doped UO_2 and (c) non-irradiated undoped UO_2. The configuration-averaged EXAFS signal was calculated by the MD-EXAFS method at T = 300 K using the core-shell potential of Meis et al.

2D scanning LIBS procedure

LIBS spectroscopy for composition profile of TOKAMAK hot wall laser pulse by by pulse ablation spectra of W, Mo, Al, H, D of the tokamak hot wall material





2D LIBS

- Ablation of single layer, performed by number of pulses covering given surface (e.g. 10 x10; 30x30 etc.) followed by data averaging;
- Layer by layer ablation of the given surface - depth profile;
- Decrease of the single layer thickness up to ~70 nm; increase of the depth profile accuracy of elements