SEMINARIUM RENTGENOWSKIE

Dnia 23.01.2018 r. o godz. 10.30, w sali D Instytutu Fizyki PAN, odbędzie się seminarium rtg., na którym **mgr Pavlo Konstantynov** z IF PAN, wygłosi referat na temat:

"Application of molecular dynamics simulations to interpret X-ray absorption spectra"

Streszczenie:

The effectiveness of classical molecular dynamics (MD) simulations for the interpretation of x-ray absorption fine structure (XAFS) of thermally activated decomposition of diluted magnetic semiconductors, namely, (Ga, Mn)As after medium temperature post growth annealing was tested. To determine the local atomic structure around Mn atoms XAFS spectra at Mn K-edge were gathered at about 90 K at BL22 beamline, ALBA synchrotron facility (Spain). The annealed samples show reorganization of the near edge electronic structure and dramatic decrease of the modulus of Fourier transforms amplitude, |FT(R)|, with annealing temperature increase. This decrease can be modeled either via (i) an increase of the Debye-Waller factor and/or (ii) a decrease of neighboring atoms number around Mn (which is a result of structural transformation caused by Mn atoms migration in GaAs matrix before formation of Mn-rich inclusions in GaAs matrix). Various models with vacancies, as well as interstitial and substitutional point defects (Mn_{Ga}, Mn_i) were studied using MD simulations to produce theoretical EXAFS/XANES signals that were then directly compared to the experimental ones. The creation of an effective model describing the local structure around manganese atoms in samples depleted at higher temperatures underwent considerable difficulties. Thus, additional studies of the investigated system were carried out using X-ray diffraction at synchrotron facility (ELETTRA, Italy). Qualitative analysis of the experimental data reveals the (Ga, Mn)As lattice parameter temperature dependence as well as retrace MnAs - type nanoinclusions created by annealing treatment in these materials and dynamics of their structure evolution with temperature. The obtained results were, then, used to model the XAFS spectra. It was found that combination of discovered by XRD secondary phase (rock salt) along with the original one (sphalerite) describes qualitatively quite well the fine structure of the X-ray absorption spectra of the samples annealed at higher temperature.

Prof. dr hab. Krystyna Jabłońska