XRD investigations combined with molecular dynamics simulations to interpret X-ray absorption spectra

P. Konstantynov[1], R. Minikayev[1], Y. Syryanyy[1], Y. Melikhov[2], J. Domagala[1], J. Sadowski[1,3], and I.N. Demchenko[1]

[1] *Institute of Physics, Polish Academy of Sciences, Lotnikow Alley 32/46, 02-668 Warsaw, Poland*
[2] *School of Engineering, Cardiff University, Cardiff, CF24 3AA, United Kingdom*
[3]*Max-IV Laboratory, Lund University, Lund SE-221 00, Sweden*

The performance 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 studied. 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 amplification. This diminution can be modeled either via (i) an increase of the Debye-Waller factor and/or (ii) a reduction 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. In such a way, using X-ray diffraction at synchrotron facility (ELETTRA, Italy), additional studies of the investigated system were carried out. These investigations have shown that annealing of the samples using the range of temperature of 350-550 ^{0}C forms the second crystal phase, which is not MnAs-hexagonal one. The deep analysis of obtained XRD pattern has shown that the second phase is a salt-rock structure. Taking into account this result, new models, based on mixing of initial sphalerite-GaAs and salt-rock structures, were created for the theoretical calculations of EXAFS spectra. The comparison of selected theoretical spectra with experimental ones, has shown relatively good agreement. Moreover, the XANES theoretical spectra based on selected/preferable models are in qualitative agreement with the experimental data.