P-04

The MD simulations for the interpretation of thermally activated decomposition of (Ga,Mn)As thin layers at medium temperature post growth annealing

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Keywords: synchrotron radiation, XAFS, molecular dynamic, DFT, FEFF

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A potential simultaneous use of the ferromagnetic and semiconductors properties in spintronics has attracted a great interest to diluted magnetic semiconductors (DMS) with the most studied material being (Ga,Mn)As. With the optimized MBE growth and post growth annealing procedures nowadays (Ga,Mn)As layers have achieved the Curie temperature, T_C, as high as about 200 K. This is remarkably high as for DMS, but still too low in view of potential application in spintronics devices. From physics point of view, an indirect coupling between localized spins mediated by charge carriers is of paramount importance for the possibility of magnetic ordering in DMS [1]. However, the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction mechanism, which is used to describe the properties of DMS systems, has limitations predicting an increase of T_C with increasing concentration of Mn impurities, the situation which is not always experimentally observed. Further studies not only on the influence of microstructure and its inhomogeneities upon material's properties but also on transformation processes (including formation and migration of point defects) which occur in (Ga,Mn)As during growth and post growth annealing should lead to an improved understanding of the microstructure evolution and could potentially lead to a further progress in reaching larger T_C in (Ga,Mn)As.

The goal of this project is to check the effectiveness of classical molecular dynamics (MD) simulations for the interpretation of x-ray absorption fine structure (XAFS) of thermally activated decomposition of DMS, namely, (Ga,Mn)As after medium temperature post growth annealing. The (Ga,Mn)As layer was grown in a SVTA MBE system [2] on GaAs (100) substrate. After growth it was cleaved into four pieces: one was left intact (as-grown) and three were annealed at 250, 350, and 450°C, respectively. Finally, the separation of the (Ga,Mn)As layer from the GaAs substrate was performed by chemical etching, a so-called "lift-off" procedure [3].

In order to determine the local atomic structure around Mn atoms the XAFS spectra at the K-edges of Mn were gathered at the BL22 CLÆSS beamline at ALBA light source [4] at LN temperature. Figure 1 presents normalized XANES spectra around Mn K edge, whereas, an inset shows modulus of Fourier transforms, FT(R), of the EXAFS function for each of the samples. The analysis of XANES spectrum of the "as-grown" sample indicates that Mn atoms most likely substitute Ga in the GaAs matrix, which is also supported by our own *ab initio* simulation results. The annealed samples show: (i) reorganization of the near edge electronic structure; together with (ii) a dramatic decrease of FT(R) amplitude with increase of the annealing temperature. Such behavior of XAFS signal is a likely indicator of a redistribution/diffusion of Mn atoms in the host matrix, which allowes us to propose the following working hypothesis: starting from the randomly distributed substitutional manganese, Mn_{Ga} (referred as monomers), and point defects like Mn_i (interstitial manganese), V_{As} or V_{Ga} (corresponding vacancies) formation of non-regular distributed areas of "*N-mers*" (dimer, trimer and so on combined through As) could occur, which eventually could lead to formation of Mn-rich (Ga,Mn)As clusters. Theoretical support of this working hypothesis comes from our *ab initio* calculations performed by WIEN2k code, as well as theoretical studies by Raebiger *et al.* [5].

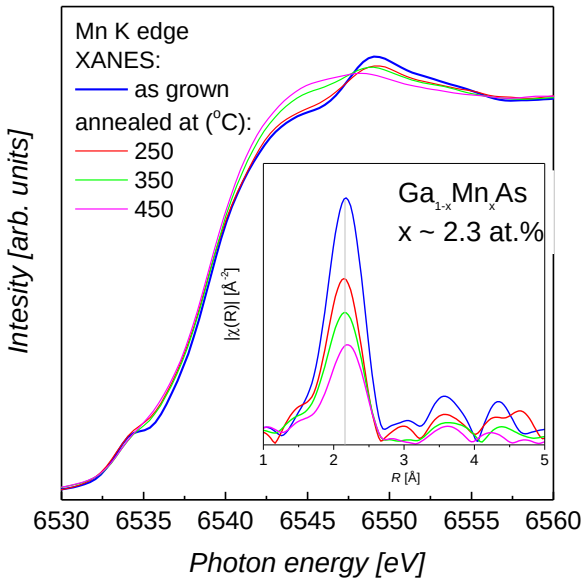

Figure 1 Normalized Mn K-edge XANES spectra of the (Ga,Mn)As layers (i.e. after the "lift-off" procedure) (The inset shows Fourier transforms of the k-weighted Mn K-edge EXAFS χ function).

Based on our working hypothesis we constructed the model structures (4x4x4 supercell) which are expected to correspond to different stages of annealing process. The NVT-type classical MD simulations using GULP code were performed where each structure was equilibrated at 90 K (the temperature of the EXAFS experiment), and a set of instantaneous atomic configurations was accumulated during the production run and averaged. XAFS spectra for each averaged atomic configuration (constructed by the FEFF code) were used to perform

qualitative/quantitative analysis of the EXAFS/XANES spectra of the annealed samples, respectively. This analysis showed that the signal is a combination of signals coming from both Mn monomers and "*N-mers*".

Acknowledgments: We acknowledge the support from the EAgLE project (Project Number: 316014) and from ICM infrastructure.

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P-05

High-resolution Powder Diffraction Study of $Ca_9R(VO_4)_7$ (R = La, Gd) Crystals

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Whitlockite is a mineral of the formula $Ca_9(MgFe)(PO_4)_6PO_3OH$ (*R*3*c* space group). Whitlockite-related materials form an extended family of compounds. Those of the $Ca_9R(VO_4)_7$ formula (R = a rare earth) are considered for applications in optoelectronics, *e.g.*, in white-light emitting diodes and lasers. In the $Ca_9R(VO_4)_7$ structure the R atoms partially occupy the Ca sites with occupation depending on the choice of the R atom. In this work, $Ca_9R(VO_4)_7$ (R – La, Gd) single crystals are studied. They were grown by the Czochralski method. The structure was refined using the powder diffraction data collected at a high-resolution synchrotron beamline. The structural details of the samples will be discussed.

P-06

Evaluation of zirconia dioxide tetragonal phase degradation introduced by grinding with dental burr

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Thanks to the evolution of CAD/CAM systems, zirconia is increasingly popular as ceramic material for dental restorations. Most often zirconia is used as modified yttria (Y_2O_3) tetragonal zirconia polycrystal (Y-TZP). Between the different ceramics utilized in dental prosthodontics, zirconia shows optimum properties: superior toughness, strength, and fatigue resistance, excellent wear properties and biocompatibility. Pure zirconia presents the phenomenon of allotropy, that is, same chemical composition but different in atomic arrangement, namely: orthorhombic, monoclinic, tetragonal, cubic, liquid. Y-TZP is a metastable material, however incorrect dental processing may induce unfavorable phase transitions, gaining more monoclinic amount and in turn, corrupting mechanical properties of the material [1,2].

The aim of the analysis was verification of the influence of dental processing protocols, on phase transition of yttrium stabilized zirconium dioxide. Evaluation of Y-TZP structure was performed with scanning electron microscopy (SEM) and X-ray diffraction (XRD). Zirconia samples were grinded with different dental burs (varies in diamond grit size) to simulate the procedures that usually the material undergoes. At the same time recorded with infrared camera for evaluation of generated temperature.

XRD study revealed impact of mechanical processing methods on the range of transition from tetragonal to monoclinic phase of the tetragonal zirconia polycrystals. The results were correlated with process accompanying generated temperature.

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