3D strain field and STEM contrast modeling of core shell nanowires containing magnetic nanoprecipitations

The 3d geometry of core-shell nanowires (NWs) with shells containing magnetic nanoprecipitations delivers new degree of freedom in design of novel type of magnetic nanoobjects. Multi shell architecture, with individual shells of different elemental composition and thickness, enables a flexible modification of the magnetic properties such a nano-object by strain and bandgap engineering. We study a 3D strain fields in NW heteostructures of “pencil like geometry”, i.e. few micrometers long wurtzite (Ga,In)As core capped by coherent epitaxial shells of (Ga,Mn)As, (Ga,Al)As with different thickness. The incoherent, semicoherent and incoherent MnAs precipitations with different size can be obtained inside the (Ga, Mn)As shell by annealing at different temperatures and by changing configuration of the shells (composition, thickness). A 3D-FEM modeling allows to study the strain state of such complex NW heterostructures. Our FE modeling is based on solving coupled problems for various fields: lattice displacements, source lattice distortions, chemical fractions, electric and/or magnetic fields. Various variants of coupling will be considered to estimate the most important effects for the residual stresses. The effect of coupling on the nucleation and formation of nanoprecipitations in the form of foreign phases are analyzed on the basis of TEM images. STEM images are calculated by means of multislice algorithm by using information about local lattice distortion obtained from 3D-FEM calculations. By comparing the experimental and simulated STEM images obtained for different camera lengths it is possible to distinguish between coherent and relaxed MnAs precipitations. This permits to perform statistic based on experimental STEM images of the number of coherent and relaxed MnAs precipitations in NW shells.

This research was co-financed by the Polish National Science Center (Grants No. 2014/13/B/ST3/0448 and 2016/21/B/ST5/03411 and by the European Regional Development Fund within the Innovative Economy Operational Programme 2007-2013 (Grant No. POIG.02.01-00-14-032/08).

Dłużewski P [1] , Wierzbicki R [1] , Tauzowski P [1] , Kret S [2] , Kaleta A [2] , Sadowski J [2,3,4]

[1] Institute of Fundamental Technological Research, Polish Academy of Sciences, ul. Pawińskiego 5 B, Warszawa, Poland

[2] Institute of Physics, Polish Academy of Sciences, al. Lotników 32/46, Warszawa, Poland

[3] MAX-IV laboratory, Lund University, P.O. Box 118, Lund, Sweden

[4] Department of Physics and Electrical Engineering, Linnaeus University, Kalmar, Sweden