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3rd International Conference on

Smart Materials & Structures

March 20-22, 2017 Orlando, USA



Rafal Kozubski

Jagiellonian University, Poland

Chemical ordering phenomena in nanostructured FePt: Monte Carlo simulations

Monte Carlo (MC) simulation studies of free-surface-induced selective destabilization of L1₀ superstructure variants in FePt nanolayers, nanowires and nanoparticles were carried out. The system was modeled with nn and nnn interatomic pair interactions deduced from ab initio results for Fe-Pt. The heterogeneous nucleation of a- and b-L1₀ variant domains reported previously for FePt nanolayers was induced by the (100)-type surfaces limiting the nanostructures. While the initial c-variant L1₀ superstructure of nanowires transformed totally to the L1₀ a-variant with Fe and Pt monoatomic planes perpendicular to the wire axis and to both (010) and (001) surfaces, in the case of nanocubes the competition between the a- and b-variant L1₀ domains nucleating at the (100), (010) and (001) surfaces resulted in suppression of their growth. As a consequence, most of the cube volume remained untransformed and showed the c-variant L1₀ chemical long-range order (LRO) with a degree lowered by homogeneously creating antisite defects. The results quantified by the calculated a- and b-L1₀ domain penetration depth and the LRO and SRO degree in particular cases are important for the development of magnetic storage media technologies requiring stable L1₀ superstructure variants determining easy magnetization directions.

Biography

Rafal Kozubski has completed his PhD from the Jagiellonian University in Kraków in 1984. He has worked as a Post-doctorate at the Strasbourg Institute of Physics and Chemistry of Materials (IPCMS), France (1987 to 1988). He was an Academic Visitor in the Institute for Applied Physics, Swiss Federal Institute of Technology, Zurich, Switzerland (1988 and 1990). He also stayed at the Institute for Solid State Physics, University of Vienna, Austria as a Lise-Meitner Fellow from 1993 to 1995. After completing his Habilitation (DSc) from the Jagiellonian University in Kraków in 1997, he has worked there as an Associate Professor (1997-2006) and in 2006, he was appointed as Full Professor at the same university. His international experience includes International Fellowship at the Queen's University in Belfast (2006-2008) and Visiting Professorships at the L.Pasteur University in Strasbourg/University of Strasbourg, France (2007, 2008, 2009, 2010 and 2011). In 2016, he was appointed as a Conjoint Professor of the University of Newcastle, Australia. He has published over 100 scientific papers in international reviewed journals and is an author of over 150 communications on international conferences.

rafal.kozubski@uj.edu.pl

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