In search of new hard magnetic materials - an experiment supported by semi-empirical calculations

Z. Śniadecki,[1] M. Kołodziej,[1,2] A. Musiał,[1] B. Idzikowski,[1] J.-M. Greneche,[3] S. Auguste,[3] M. Zubko,[4,5] and L. Bessais[6]

[1] *Institute of Molecular Physics, Polish Academy of Sciences, Mariana Smoluchowskiego 17, 60-179 Poznań, Poland*

[2] *NanoBioMedical Centre, Adam Mickiewicz University, Wszechnicy Piastowskiej 3, 61-614 Poznań, Poland*

[3] *Le Mans Universit, Institut des Molécules et Matériaux du Mans IMMM, UMR CNRS 6283, Avenue Olivier Messiaen, 72085 Le Mans, Cedex 09, France*

[4] *Institute of Materials Engineering, Faculty of Science and Technology, University of Silesia, 75 Pułku Piechoty 1a, 41-500 Chorzów, Poland*

[5] *Department of Physics, Faculty of Science, University of Hradec Králové, Rokitanského 62, 500 03, Hradec Králové, Czech Republic*

[6] *Universite Paris Est Creteil, ICMPE, UMR CNRS 7182, 2 rue Henri Dunant, 94320 Thiais, France*

The development of hard and semi-hard magnetic materials is driven by the continous growth of the global market of permanent magnets. Although it is always possible to manufacture new systems with improved properties, there is a group of metastable phases that are difficult to synthesize. Several methods are used to determine the optimal compositions, not only to improve magnetic performance but also structural stability. A relatively simple and affordable approach based on the semi-empirical Miedema's model with various modifications and extensions will be discussed. This approach is useful to mimic the synthesis process, where various intermetallic phases, the solid solution, and the glassy state compete.

The results of calculations will be presented together with the experimental evidence for various groups of alloys, *e.g.* (Hf,Cr)-Co-B system, for which the synthesis route involving rapid quenching and isothermal annealing of an initially amorphous precursor has been proposed. Another group of alloys that crystallize in a tetragonal $ThMn_{12}$-type (space group $I4/mmm$) structure and are based on Fe and rare earth elements is considered to have a potential to bridge the performance gap between ferrite and Nd-based magnets. Their progress is also hindered by low structural stability, compared to other phases competing in the synthesis process, *e.g.* Th_2Zn_{17}-type. The enthalpies of formation of the different phases in (Zr, Nd, Ce)-Fe-Si systems will be presented with a focus on the Fe-rich compositions to analyze the stability range and to propose stabilization routes.