[MS26 - 02] Phase Transformations on Nanometre Scale.

David Rafaja, Christina Wüstefeld, Christian Schimpf and Mykhailo Motylenko.

Institute of Materials Science, Freiberg University of Technology, Freiberg, Germany.
E-mail: rafaja@ww.tu-freiberg.de

Nanostructured materials play an increasingly important role in modern applications, because the materials design on the nanometre scale allows good intrinsic materials properties to be additionally improved through the manipulation of the real structure of the material. One prominent example of the nanostructured materials are multiphase nanocomposites. One way how to prepare multiphase nanocomposites with the particle size of about 10 nm or even smaller is to employ controlled phase transformations on the nanometre scale in order to fragment originally larger particles to the desired size [1, 2]. In this contribution, it will be shown how the crystallography in conjunction with X-ray powder diffraction and transmission electron microscopy can help to predict and to understand the phase transformations on nanometre scale and to explain the effect of the local strain fields in nanocomposites on the thermodynamic stability of the participating phases and/or on the stabilisation of metastable phases [3]. On the example of physically vapour deposited transition metal nitride thin film nanocomposites with addition of aluminium, (*TM*,Al)N, different phase transformation paths will be discussed, which are based on the topotactic transition, and additionally preceded or accompanied by spinodal decomposition of a metastable supersaturated solid solution. It will be shown that the kinetics of the above phase transformations is strongly influenced by the local strain fields (and thus by the local lattice deformations) emerging at the microstructure defects as well as at the crystallite and phase boundaries. The local strain fields at the crystallite and phase boundaries, which are the most important microstructure features in the (*TM*,Al)N nanocomposites and which are directly influenced by the lattice misfit at the internal interfaces, were concluded from the mutual orientation relationships of the neighbouring nanocrystallites, from the phase composition and from the distribution of the phases in the nanocomposites, and verified by the residual stress and microstrain measurements. On the example of high-pressure and high-temperature synthesised boron nitride nanocomposites, the occurrence of expected orientation relationships between individual boron nitride phases and their preservation during the phase transition of graphitic BN to sphaleritic BN over wurtzitic BN will be shown. The effect of the semicoherent interfaces, which are often formed during topotactical phase transformations, on the hardness of the nanocomposites will be discussed.

[1] Rafaja, D., Klemm, V., Motylenko, M., Schwarz, M.R., Barsukova, T., Kroke, E., Frost, D., Dubrovinsky, L. & Dubrovinskaia, N. (2008). *J. Mater. Res*. 23 (4) 981-993.
Rafaja, D., Wüstefeld, C., Motylenko, M., Schimpf, C., Barsukova, T., Schwarz, M.R. & Kroke, (2012). *Chem. Soc. Rev*. 41 5081-5101.
Rafaja, D., Wüstefeld, C., Baehtz, C., Klemm, V., Dopita, M., Motylenko, M., Michotte, C., Kathrein, (2011). *Metal. Mater. Trans. A* 42 (3) 559-569.

Keywords: metastable phases; X-ray powder diffraction; high-resolution transmission electron microscopy