Real structure analysis of nanocrystalline and submicrocrystalline materials using X-ray diffraction, Zdeněk Matěj,* Viktoria Cherkaska and Radomír Kužel, *Department of Electronic Structures, Faculty of Mathematics and Physics, Charles University in Prague, Ke Karlovu 5, 121 16 Praha 2, Czech Republic*. E-mail: matej@karlov.mff.cuni.cz

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Physical properties of nano- and submicro-crystalline materials are attractive object of study for research and industry development. Small size of coherently scattering domains and presence of lattice defects is the well-known reason of diffraction line broadening. Conventional way of X-ray line broadening analysis is based on integral breadths β or FWHMs (Williamson-Hall plot) or on Fourier coefficients (Warren-Averbach method). Description of line broadening can be phenomenological or it can be connected to a model of material microstructure. Single line Fourier coefficients as well as whole powder diffraction pattern can be calculated from such phenomenological or microstructure models. The anisotropic broadening, asymmetry and shift of diffraction lines can be accounted by a microstructure model. Simple shape (sphere, cube) of grains and lognormal distribution of their size is assumed in most cases. The Wilkens model of restrictedly random dislocations can describe deformation component of line broadening. Parameters of this model (dislocation density ρ and a R_e parameter describing dislocation correlation) and usually also two parameters of the size effect model can be determined and refined by the analysis of measured diffraction patterns. An interesting way of diffraction pattern analysis is represented by new methods based on the whole power pattern fitting [1], [2] (WPPM - introduced by the group of P. Scardi) and the multiple whole profile and Fourier coefficients fitting [3], [4] (MWP-fit - by team of T. Ungár). These methods are still in progress and authors of these methods are developing applicable software (PM2000 [1], [2], MWP-fit [3], [4]). New methods and relevant programs (MWP-fit and PM2000) are applied to nano- and submicro-crystalline samples of copper, iron and germanium obtained by high-pressure torsion deformation. Results of new and traditional methods are compared and potential of the X-ray analysis in the study of microstructure of nanocrystalline materials is demonstrated. It is shown that new methods of line profile analysis can reliably separate the size and strain broadening. The main problem is a correlation of two size parameters and especially the dislocation density ρ and the cut-off radius parameter R_e. Improvement of microstructural model for description of nanocrystalline materials obtained by severe plastic deformation is desirable. All measurements were realized on common laboratory diffractometers and hence for some methods (program MWP-fit, Warren-Averbach method) diffraction data deconvolution [5] was necessary.

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