

MS43-P05 | INVESTIGATION OF THE NANOSTRUCTURED MATERIALS BY XRD METHOD WITH USE OF SIMULATION

Cherepanova, Svetlana (Novosibirsk State University, Novosibirsk, RUS)

Nanostructured materials are specific objects of the structural analysis. Peculiarities of their X-ray diffraction (XRD) patterns arise from the presence of planar defects and/or coherently connected domains, which are elements of nanostructure. Such disordering of 3D periodic crystal structure gives rise to the diffuse scattering both in the vicinity of Bragg maxima (broadening of peaks, their shift and splitting) and/or in background region (appearance of diffuse peaks or halo). This complicates or even makes impossible the application of the traditional techniques of structural and microstructural analysis. Simulation of the XRD patterns on the base of the models of partially disordered crystals allows us to analyse all diffraction effects. It will be shown what peculiarities arise on the XRD patterns due to twinning as well due to formation of coherently connected domains having 1) the same structure, 2) the same composition but different structure, 3) different structure. Various structural types will be considered.