Structure of Nanocrystals by the Atomic Pair Distribution Function Technique

VALERI PETKOV, Dept. of Physics, Central Michigan University, Mt. Pleasant, MI 48859 — Knowledge of the atomic-scale structure is an important prerequisite to understand and predict the properties of materials. In the case of crystals it is obtained from the positions and the intensities of the Bragg peaks in the diffraction data. However, many materials of technological importance, in particular nanophase materials, are not perfect crystals. The diffraction patterns of such materials show only a few Bragg peaks and a pronounced diffuse component. This poses a real challenge to the usual techniques for structure determination. The challenge can be met by employing the so-called atomic pair distribution function technique. The basic features of the technique will be introduced and its potential demonstrated with results from recent structure studies of V$_2$O$_5$ nanotubes.

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