

EVALUATION OF SUBSTRUCTURE PARAMETERS BY PEAK PROFILE ANALYSIS OF HIGH-RESOLUTION NEUTRON DIFFRACTION SPECTRA

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The peak profile shape analysis has been preferentially used in evaluation of X-ray and synchrotron powder diffraction spectra. However, neutron diffraction facilities of new generation frequently offer the instrumental resolution high enough to study efficiently the effects of broadening of neutron diffraction profiles. Moreover, high penetration ability of neutrons enables us to use a large variety of sophisticated sample environments at neutron diffraction instruments, such as deformation machines, furnaces, cryostats, high-pressure cells, etc. These features make the high-resolution neutron diffraction instruments an unique experimental tool especially for *in situ* studies.

The present paper describes the procedure for a detailed evaluation of Bragg peak shape based on the method of transformed model fitting (TMF) which has been recently developed particularly for treatment of neutron diffraction profiles. Microstructure modeling is performed in the reciprocal space and the convolution of the model with the instrumental resolution curve is fitted to the profiles recorded in the diffraction experiment. The practical application of the TMF procedure will be demonstrated at the study of evolution of microstructural parameters of the ferritic steel *in situ* upon tensile straining. In this case, the Wilkens dislocation model and a log-normal crystallite size distribution were implemented into the model of the line broadening.