

Modeling the effect of the core region of dislocations to X-ray or neutron diffraction patterns

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X-ray Line Profile Analysis

Diffuse scattering

Microstructure modeling

Abstract

Crystalline materials produce broadened X-ray or neutron diffraction peaks corresponding to the Bragg positions. Alloys, compounds, structural or complex solid materials are never free from defects. By analyzing the broadening of the peaks using the method of line profile analysis one can obtain information about microstructure, including coherently scattering crystallite size, defect types and defect densities. However, observed diffraction patterns can have more complex structures. It is not only a set of Bragg peaks, but also the regions far from the center of peaks and below the peaks can hold important information about the microstructure. These regions can be better observed by using logarithmic intensity scale. There are different physical reason causing these features. Small coherent precipitates, Guinier-Preston (GP) zones or irradiation induced small dislocation loops can produce satellite peaks attached to the main diffraction peaks of the matrix material [1,2]. Satellites can be modelled and separately analyzed in terms of misfit, crystallite size or strain distribution [3]. When the crystal defects are small or not perfectly crystalline, they produce slowly varying diffuse scattering below the Bragg peaks.

The total diffraction consisting of Bragg peaks and diffuse scattering underneath them can be analyzed separately. The diffuse scattering contribution can be related to a variety of materials components, e.g. to amorphous or short range order regions, or to point defects etc. [4,5]. Based on the observation that severely plastically deformed materials containing a high density of dislocations have significant diffuse scattering components below the Bragg peaks the authors developed a model taking into account the diffuse scattering part as the contribution of the disordered lattice near the core region of the dislocations. The model describes well the observed pattern as the sum of a smooth simple background function, the broadened Bragg peaks and the satellite peaks which correspond to the core regions of the dislocations which have a significant volume fraction in these cases.

References

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