Chapter 8
X-Ray Line Profile Analysis for Single Crystals

ABSTRACT

The features of the dislocation structure in plastically deformed single crystals can be determined from diffraction line broadening. Both the measuring and the evaluation procedures of X-ray line profiles are somewhat different from the methods used for polycrystalline materials. In this chapter, these procedures are overviewed, and their effectiveness is illustrated by representative examples. It is shown that the intensity distribution in the vicinity of the reciprocal lattice points can be mapped by rocking the single crystal about appropriate axes. From the detected intensity distribution, the density, the slip systems, and the arrangement of dislocations, as well as the lattice misorientation can be determined. The average misorientation obtained from rocking curve measurement can be related to the density of geometrically necessary dislocations. It is also shown that the inhomogeneous distribution of dislocations in plastically deformed single crystals usually results in asymmetric line profiles. The evaluation of these peaks enables the determination of the long-range internal stresses besides the dislocation densities in the dislocation cell walls and interiors.

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INTRODUCTION

In a single crystal the broadening of line profiles is caused by the lattice defects. Since for a measurable broadening long-range internal stresses are needed, therefore the line profile analysis in single crystals mostly deals with the characterization of the dislocation structure formed during plastic deformation. Both the density and the arrangement of dislocations can be determined from the shape and breadth of peak profiles. However, the measurement and the evaluation of diffraction line profiles in single crystals are somewhat different from the procedures applied for polycrystalline materials. For instance, the diffracted intensity for the different reflections can only be measured in specific orientations of the sample. Therefore, if the different slip systems are not populated equally by dislocations, the dislocation contrast factors averaged for all slip systems can not be used in line profile analysis (see chapter 3). Additionally, the intensity distributions around the reciprocal lattice points in the different directions reflect various features of the microstructure. The intensity profile parallel to the diffraction vector depends on the density and arrangement of dislocations (Mughrabi, Ungár, Kienle, & Wilkens, 1986; Székely, Groma, & Lendvai, 2001), while the intensity distribution perpendicular to the diffraction vector is correlated to the misorientations caused by the dislocation boundaries formed in the single crystal (Wilkens, Ungár, & Mughrabi, 1987; Mughrabi & Obst, 2005). In the following, the correlation between the dislocation structure and the diffraction peak broadening for single crystals is overviewed. Special attention is paid to the evolution of asymmetry of line profiles caused by the long-range internal stresses remained after plastic deformation.

INTENSITY DISTRIBUTION AROUND THE RECIPROCAL LATTICE POINTS FOR SINGLE CRYSTALS

The intensity distribution in the reciprocal lattice node with the indices *hkl* for a single crystal is illustrated in Figure 1. The broadening along the reciprocal lattice vector (or diffraction vector) $\boldsymbol{g}_{hkl}$ corresponds to the variation of the lattice spacing for planes (*hkl*) due to the strain fields of dislocations. The broadening perpendicular to $\boldsymbol{g}_{hkl}$ represents the variation of the orientations of lattice planes (*hkl*) with respect to a reference orientation (Mughrabi & Obst, 2005). The former and latter broadenings are referred to as line broadening and broadening of rocking curve, respectively. The rocking curve is measured with a fixed detector position at the Bragg angle corresponding to reflection *hkl*, while the sample is rotated about the axis perpendicular to the plane of the incident and the diffracted beams (referred to as rocking axis). In this procedure the head of the diffraction vector scans an arc centered at

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