Chapter 3
Strain Broadening of X-Ray Diffraction Peaks

ABSTRACT

The line shape caused by lattice distortions in a crystal is reviewed. It is revealed that the broadening of a diffraction peak with indices hkl is related to the mean-square-strain perpendicular to the reflecting (hkl) lattice planes. The strain broadening of line profiles depends on the order of diffraction. The line profiles for a crystal in which the lattice distortions are caused by dislocations are described in detail in this chapter. It is revealed that the anisotropic strain field of dislocations yields a special dependence of peak broadening on indices of reflection. The stronger the screening of the strain fields of dislocations, the longer the tails in the diffraction profiles. For polarized dislocation walls, the diffraction peak is asymmetric, and the antisymmetric component of the profile is determined by the dislocation polarization. It is shown that the strains in nanoparticles resulted by the relaxation of their surfaces also lead to line broadening.

INTRODUCTION

X-ray diffraction lines are broadened if the atomic positions do not follow the order characteristic of the crystal structure. The displacements from the ideal atomic positions are referred to as lattice distortions. Lattice distortions are usually caused by the strain fields of lattice defects. The strain field of a point defect, such as a vacancy or an interstitial atom, decreases with r^{-3}, where r is the distance from the defect, therefore it decays very quickly with increasing r and does not yield detectable broadening of X-ray line profiles. At the same time, the strain field of an individual dislocation is of long-range character as it decays with r^{-1}. Due to the reciprocity between crystal

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and reciprocal spaces, the scattering related to point defects (referred to as Huang scattering) is extended far from the fundamental Bragg reflections and therefore not involved in the evaluation of line profiles (Trinkaus, 1972). Due to the long-range character of strain field of dislocations, these defects yield considerable broadening of line profiles (Krivoglaz, 1969; Wilkens, 1987). Dislocations are important lattice defects in crystalline materials as they play a unique role in plastic deformation, especially in metals and alloys. In addition to lattice defects, there are other sources of lattice distortions. For instance, in nanoparticles the surface relaxation causes displacement of atoms from their ideal positions which leads considerable diffraction peak broadening due to the large volume fraction of surface shell in nanosized crystallites (Leoni & Scardi, 2002; Leoni & Scardi, 2004). In this chapter, the X-ray line profiles resulted by lattice distortions are reviewed with special attention to the peak broadening caused by dislocations.

GENERAL EFFECT OF LATTICE DISTORTIONS ON LINE PROFILES

The atomic positions in a real crystal deviate from a perfect order as the external and/or internal stresses yield displacement of atoms from their ideal positions. These lattice distortions are usually caused by lattice defects, such as dislocations, but they may have other sources such as surface relaxation in nanoparticles. The displacement of lattice points from their ideal positions may cause both shift and broadening of the diffraction peaks. The first and the second effects are related to the change of the average spacing between atoms due to stresses and the variance in the interatomic spacing, respectively. In order to separate these two effects, we will introduce the concept of the ideal average lattice (Guinier, 1963). First, let us imagine an ideal crystal with perfect atomic order (see Figure 1a). Then, displace the lattice points (atoms) away from their theoretical positions as shown in Figure 1b. It is noted that in a real crystal the displacements are small compared to the interatomic spacings. An ideal average lattice can be constructed throughout the crystal for which the vectorial sum of the atomic displacements is zero, i.e. $\sum_i \boldsymbol{u}_i = 0$ (Guinier, 1963). The ideal average lattice is illustrated by dashed lines in Figure 1c. Then, the diffraction peak shifts can be obtained by the difference in lattice spacings between the original and the average crystals, while the diffraction line broadening can be related to the displacements in the ideal average lattice. The strain causes peak shift or line broadening is usually referred to as macro- or microstrain, respectively. In the following, we will deal only with the description of the peak profile broadening caused by the lattice distortions.