Chapter 7
Peak Profile Evaluation for Thin Films

ABSTRACT

The special phenomena in X-ray diffraction line profile analysis occurring in thin films is overviewed in this chapter. In the case of textured nanocrystalline thin films, the line broadening caused by the crystallite size increases with the length of the diffraction vector. This effect is explained by the interference of X-rays scattered coherently from adjacent crystallites with close orientations. The partial coherence of adjacent nanocrystallites is caused by the overlapping of their reciprocal lattice points. The smaller the size and the stronger the orientation preference of crystallites, the better the coherence. This interference effect yields narrowing of line profiles at small diffraction angles, while it has no influence on line broadening at large angles. Therefore, the traditional line profile evaluation methods give much larger crystallite size than the real value and may detect a false microstrain broadening. Some ways for the correction of the interference effect are proposed. Detailed case studies are given for the determination of the defect structure in thin films by line profile analysis.

INTRODUCTION

Lattice defects (e.g. grain boundaries, dislocations and planar faults) in polycrystalline thin films are crucial for their properties, such as for the yield strength of hard foils or critical current density under magnetic field in high temperature superconducting multilayers. Therefore, the determination of the crystallite size as well as the defect types and densities is strongly recommended in the studies of foils and coatings. X-ray diffraction peak profiles analysis has been successfully applied for the determina-

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tion of the types and the densities of different lattice defects. For instance, Csiszár, Li, Zilahi, Balogh, and Ungár (2013) have shown by line profile analysis that the reduction of the dislocation density during oxygenation of $GdBa_2Cu_3O_{7-x}$ multilayers is a necessary condition to obtain superconductivity. Kuzel Jr, Cerny, Valvoda, Blomberg, Merisalo, and Kadlec (1995) have studied magnetron sputtered TiN thin films with different porosities and revealed that in porous films the line broadening caused by the small crystallite size is dominating, while in compact layers the effect of microstrain caused by dislocations prevails. The lattice defect structure in thin films is also influenced by the substrate, as shown for ZnO foils (Kuzel, Cizek, & Novotny, 2012). Misfit dislocations in thin layers generally form in order to relax the stresses induced by the mismatch between the lattices of the foil and the substrate. Kaganer, Köhler, Schmidbauer, and Opitz (1997) have calculated the X-ray peak intensity distribution caused by different arrangement of misfit dislocations and successfully explained the experimentally measured shapes of line profiles for the following pairs of layer/substrate: AlAs/GaAs, $Si_{1-x}Ge_x$/Si, AlSb/GaAs and InAs/AlSb. Due to the small thickness of thin films their microstructures are often studied by other experimental methods than the conventional powder diffraction technique (Kuzel Jr, Cerny, Valvoda, Blomberg, & Merisalo, 1994). For instance, if a thin film is investigated on the substrate, a glancing-angle X-ray diffraction geometry is preferred in order to suppress the signal of the substrate and improve the scattering from the foil by reducing the penetration depth and increasing the length of X-ray path through the film, respectively (Friedbacher & Bubert, 2011). The glancing-angle geometry with parallel beam is illustrated in Figure 1. The incident parallel beam is obtained by a Goebel mirror inserted in the primary radiation. Due to the very small incidence angle, ω, (typically under 2°) the penetration depth is usually between 10-1000 nm (Matej, Nichtova, & Kuzel, 2009). The penetration depth is nearly independent of the diffraction angle (i.e. of the indices of reflection), however it can be varied by changing the incidence angle of the X-ray beam to sample surface (Kuzel Jr, Cerny, Valvoda, Blomberg, & Merisalo, 1994). At incidence angles close to the angle of total reflection (e.g. $\omega_c = 0.28°$ for TiO_2) the penetration depth is only a few nanometers. Due to the small incidence angle the irradiated area on the film surface is large, therefore the diffracted beam is wide which usually yields several times worse peak profile resolution than in the case of focusing Bragg-Brentano geometry. However, if the foil is removed from the substrate before X-ray measurements, the usual diffraction geometries can also be applied for thin films.

The microstructure of polycrystalline thin films usually deviates considerably from their bulk polycrystalline counterparts due to the strong texture (Rafaja, Poklad, Klemm, Schreiber, Heger, Sima, & Dopita, 2006) and/or the preferred orientation of lattice defects relative to the foil surface (Nyilas, Misra, & Ungár, 2006; Csiszár, Misra, & Ungár, 2011; Csiszár, Pantleon, Alimadadi, Ribárik, & Ungár, 2012). The strong texture may lead to a coherent scattering of adjacent crystallites which results

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