A Novel Diffraction Technique to Determine Mechanical Moduli of Fibre-Textured Thin Films

K.J. Martinschitz and J. Keckes
Erich Schmid Institute for Materials Science, Austrian Academy of Sciences and Institute of Metal Physics, University of Leoben , Leoben, Austria

A determination of elastic constants of thin films with the thickness in the nm range represents a serious difficulty. The purpose of this contribution is to introduce a *new self-consistent diffraction technique* that allows for a rapid experimental determination of in-plane Young's modulus and Poisson's number of thin films by X-ray diffraction. The mechanical elastic constants are extrapolated from thin film X-ray elastic constants considering specific sample anisotropy. The X-ray elastic constants can be determined by a simultaneous application of $\sin^2\psi$ and X-ray diffraction substrate curvature techniques. The basic idea resides in the fact to use a monocrystalline substrate with known mechanical properties as an internal standard to determine the relationship between the measured X-ray elastic strains and the macroscopic stress. The macroscopic stress imposed on a film which is deposited on a mono-crystalline substrate can be calculated from the substrate curvature using Stoney's formula. The curvature is determined by the measurement of rocking curves on the substrate symmetrical reflections at different sample positions. This gives an opportunity to characterize the X-ray elastic strains for different *hkl* reflections and also the curvature of the substrate in one XRD system without remounting the sample. The knowledge of the macroscopic stress and the elastic strains can then be used to quantify X-ray elastic constants for different *hkl* reflections. In order to extrapolate mechanical elastic constants from X-ray elastic constants, however, it is necessary to consider the preferred orientation in the thin film. One of the main goals of this contribution is to demonstrate for which *hkl* reflection (and the value of the anisotropic factor Γ) the X-ray elastic constants are equal to their mechanical counterparts. This analysis is made by comparing calculated mechanical and X-ray elastic constants of thin films possessing various orientation distribution function $f(g)$. At the end a certain type of a selection rule will be presented.
The new approach is demonstrated on a variety of thin film systems like TiN, CrN, Al, Cu deposited on Si(100) wafers and measured using laboratory and synchrotron source (BESSY and Hasylab) at room and at high temperatures up to 600°C.
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