

Direction-dependent grain interaction in nickel and copper thin films, analysed by X-ray diffraction

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Abstract

The elastic grain interaction due to surface anisotropy and morphological ('grain-shape') texture in real, polycrystalline materials has been considered. It has been demonstrated for the first time that the effect of surface anisotropy and morphological texture on polycrystal elastic behaviour can be distinguished in a diffraction stress analysis by evaluating lattice strain measurements from multiple reflections *simultaneously*. Non-linear $\epsilon\text{-}\sin^2\psi$ plots (i.e., plots of the lattice strain ϵ versus $\sin^2\psi$, where ψ is the angle between the surface normal of the specimen and the diffraction vector) have been obtained for 001 and *hhh* reflections in the diffraction stress analysis of sputter-deposited nickel and copper thin films. Such observed non-linearities can only be interpreted on the basis of a direction-dependent grain interaction due to surface anisotropy or morphological (grain-shape) texture. For the specimens investigated, it has been found that surface anisotropy is the dominant factor causing the observed non-linearities in the $\epsilon\text{-}\sin^2\psi$ plots. These findings have been confirmed by focused ion beam microscopy: The specimens investigated do not exhibit a grain-shape texture.

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1. Introduction

For a single crystal, the elastic strain due to applied stress can be calculated straightforwardly from Hooke's law. If, however, the crystal is embedded as a grain in a polycrystalline body, it is surrounded by differently oriented neighbouring grains and, if intrinsic (single-crystal) elastic anisotropy occurs, due to the interaction of the grains, constraints occur for the strain upon applied stress in the grain considered. The so-called elastic grain interaction models describe the distribution of stresses and strains over the crystallographically differently oriented grains of a mechanically stressed polycrystal. They allow the calculation of mechanical elastic constants and diffraction (X-ray) elastic constants (diffraction (X-ray) stress factors for macroscopically elastically anisotropic samples), which

relate the lattice strains as measured by diffraction to the mechanical stress [1].

Traditionally, isotropic grain interaction models are considered: identical (i.e., 'isotropic') grain interaction constraints prevail along all directions in the specimen. Examples of isotropic grain interaction models are provided by the classic Voigt [2], Reuss [3] and Eshelby–Kröner [4,5] models. Polycrystals exhibiting isotropic grain interaction are macroscopically elastically isotropic in the absence of crystallographic texture, but macroscopically elastically anisotropic if texture occurs¹ [1].

Only recently, the so-called direction-dependent grain interaction models have been proposed [1,6–10]. The notion of 'direction-dependent grain interaction' signifies that different grain interaction constraints prevail for different directions in the specimen. Polycrystals exhibiting

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¹ In the following, the notion texture without further specification refers to the occurrence of crystallographic not morphological (grain-shape) texture.

direction-dependent (i.e., anisotropic) grain interaction are macroscopically elastically anisotropic, also in the absence of texture [1].

Two cases of direction-dependent (anisotropic) grain interaction can be distinguished: surface anisotropy and a morphological texture.

Surface anisotropy. In an infinitely large bulk polycrystal, each grain is surrounded by neighbouring grains in three dimensions. In a (columnar) thin film or the surface layer of a bulk polycrystal, in contrast, each crystallite is surrounded by neighbouring crystallites in only two dimensions. The grain interaction perpendicular to the surface can thus be different from the grain interaction parallel to the surface: direction-dependent (anisotropic) grain interaction occurs [10]. To deal with the effect of surface anisotropy on the elastic behaviour of polycrystals, the so-called Vook–Witt and inverse Vook–Witt grain interaction models have been introduced and an effective grain interaction model has been proposed [6,7,11].

Morphological texture. It may be expected that an anisotropic, direction-dependent grain interaction in general can occur in polycrystals with a macroscopically anisotropic microstructure. It can thus be anticipated that polycrystals composed of non-spherical grains with their principal (shape) axes aligned more or less preferentially along certain directions in the specimens (i.e., a grain-shape or morphological texture occurs) exhibit macroscopically elastically anisotropic behaviour, i.e., direction-dependent grain interaction occurs. The effect of a grain-shape texture on the mechanical elastic constants and the diffraction stress factors can be modelled employing an extension of the traditional Eshelby–Kröner model [4,5]. A detailed outline of the theoretical background and the calculation scheme has been given previously [9].

Diffraction analysis is a very sensitive tool for investigating the direction-dependent grain interaction, because both the spatial variation of the (lattice) strain and its (hkl) specificity are analysed, where the grain interaction is expressed by the so-called diffraction elastic constants (diffraction stress factors for macroscopically elastically anisotropic specimens), which represent the elastic response for only the diffracting material [1]. The macroscopic mechanical elastic constants represent the elastic response for the whole body and, accordingly, in general are significantly less dependent on the type of grain interaction occurring [6,7].

Traditionally, two cases have been distinguished in diffraction stress analysis: crystallographically untextured specimens and crystallographically textured specimens. Linear (or elliptic, in the presence of shear stresses) plots of the lattice strain versus $\sin^2\psi$, where ψ is the inclination of the diffraction vector with respect to the surface normal of the specimens, are expected for crystallographically untextured specimens. Curved plots are expected for textured specimens [12]. Exceptions are the 001 and hhh reflections of specimens consisting of cubic materials, which are expected to exhibit linear $\sin^2\psi$ plots also in

the presence of texture (e.g., see Refs. [12,13]). Recently, it has been demonstrated on a rigorous mathematical basis that linear (or elliptic) $\sin^2\psi$ plots occur for macroscopically elastically isotropic specimens, whereas non-linear $\sin^2\psi$ plots occur for macroscopically elastically anisotropic specimens [1]. Straightforward diffraction evidence of direction-dependent grain interactions is thus obtained if deviations of straight-line behaviour occur in $\sin^2\psi$ plots of untextured specimens or in $\sin^2\psi$ plots for the 001 and hhh reflections of crystallographically textured specimens of cubic materials.

Indeed this is the line of reasoning followed by van Leeuwen et al. [10] in their pioneering work demonstrating the occurrence of a direction-dependent grain interaction in an untextured stressed thin film. Subsequently, grain interaction models accounting for surface anisotropy have been employed in a few investigations [6,7,14]. There is a lack of experimental studies on the effect of grain-shape texture and on distinguishing between the various types of anisotropic grain interaction.

In this work the grain interaction in sputter-deposited nickel and copper layers has been investigated by X-ray diffraction. It is shown for the first time that the simultaneous analysis of lattice strain data obtained from multiple reflections (i.e., the simultaneous use of multiple $\sin^2\psi$ plots) allows identification of the kind of (anisotropic) grain interaction relevant for the specimen under investigation. The results obtained for the grain interaction are discussed in the light of the microstructures of the specimens as observed using focused ion beam (FIB) microscopy.

2. Theoretical basis

2.1. Surface anisotropy

Extreme types of isotropic grain interaction are given by the so-called Voigt [2] and Reuss [3] models: all directions in the specimen frame of reference are equivalent with respect to grain interaction. In the Voigt model it is assumed that the strains in the specimen frame of reference S are equal for all crystallites. In the Reuss model, in contrast, it is assumed that the stresses in the specimen frame of reference S are equal for all crystallites in the sample.

Models for the anisotropic grain interaction in a (columnar) thin film or the surface layer of a bulk polycrystal take into account that a grain is surrounded by neighbouring grains in only two dimensions: the interaction parallel to the surface/layer and the interaction perpendicular to the surface/layer are distinguished. There are two grain interaction models of extreme types of grain interaction assumptions for bulk materials (see above: Reuss and Voigt models). Four types of extreme grain interaction models then can be formulated for (columnar) thin films (and surface regions of bulk materials), as there are two principal directions, each with two extreme types of grain interaction (i.e., Reuss and Voigt type of grain interaction). These four extreme grain interaction models are the Reuss,

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