MICROMECHANICAL MODELLING OF ELASTIC THIN FILMS AND COMPARISON WITH IN SITU TENSILE TEST WITH XRD MEASUREMENT

G. Geandier[a,b], O. Castelnau[a] , L. Thilly[b], E. Le Bourhis[b], P.-O. Renault[b], Ph. Goudeau[b]
[(a)] LPMTM – CNRS, Paris XIII, 99 Avenue Jean-Baptiste CLEMENT F-93430 VILLETANEUSE
[(b)] *PhyMat – UMR 6630- SP2MI, BP 30179 - 86 962 FUTUROSCOPE CHASSENEUIL cedex*

Our aim is to determine the elastic modulus softening for poly-crystalline materials with nanometric grain size. The use of metallic multilayers materials deposited as thin films permit to control the deposition process, the grain size and the sample microstructure. We used X-rays diffraction experiments coupled with in situ tensile test to determine the Bragg peaks displacements for several {hkl} planes, crystalline orientations and for the different films constituents. A micro-mechanical model was developed for results interpretations. There are two levels of heterogeneities in the material. Macroscopic applied stress is distributed between the layers as a function of their effective modulus, the stiffer layers supporting higher stresses. Then, inside the layers, stress is not homogeneously distributed because of the elastic anisotropy at the grain scale, and as for the layers, stress is located at the "stiffer grains". The micro-mechanical model presented here is developed to take into account the structure of each layer on the displacement of the peaks obtained by X-ray diffraction [1]. More precisely, we calculate the inter-granular interactions inside each layer with an homogenization method in mean field. For bulk poly-crystals, the self consistent model (SC) is generally adopted and gives results in good agreement with experimental determinations and with other calculations methods in full field [2]. This model gives the exact effective behavior for some random microstructures. In a first time, we adopt the same formalism for poly-crystals in thin layer as considered here, with encouraging results from Faurie and al [3]. Then we propose to use some results from literature in order to estimate the effective behavior of a multilayer material. When the layers show a homogeneous elastic behavior, if the interfaces are perfect (plane and parallel), the exact results can be expressed easily. This model with two scale changes, from grain to layer and from layers to multilayers, permit to take into account of the microstructure (texture, crystallography, ...) of each layer in the estimation of the stress and elastic strain distributions at the layer and grain scales.
The results is compared to experimental data collected during a campaign at the ALS (Berkeley National Lab.) with in situ tensile test in the elastic domain. Comparison between experimental data and model is very good, showing the model aptitude to reflect the stresses localisation in the different films constituents. The global agreement associated with the proposed model (allowing very fast numerical resolution) opens the opportunities to use this model in an inverse way to estimate the elastic modulus softening for materials with low dimensions.

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[2] Lebensohn R.A., O. Castelnau, R. Brenner, P. Gilormini, Int. J. Solids Struct. **42**, p.5441-5459, 2005.
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Speaker name : Ludovic Thilly
Laboratoire de Physique des Matériaux – UMR 6630- Université de Poitiers – UFR Sciences
SP2MI, Boulevard M&P Curie - BP 30179 - 86 962 FUTUROSCOPE CHASSENEUIL cedex
ludovic.thilly@univ-poitiers.fr
tel : 33-549496831
fax : 33-549496642

Corresponding person : Guillaume Geandier
Laboratoire de Physique des Matériaux – UMR 6630- Université de Poitiers – UFR Sciences
SP2MI, Boulevard M&P Curie - BP 30179 - 86 962 FUTUROSCOPE CHASSENEUIL cedex
guillaume.geandier@univ-poitiers.fr
tel : 33-549496731
fax : 33-549496642

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