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Hamidreza Abdolvand, Jonathan P. Wright, Angus J. Wilkinson

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On the state of deformation in a polycrystalline material in three-dimension: elastic strains, lattice rotations, and deformation mechanisms

[1,3]Hamidreza Abdolvand, [2]Jonathan P Wright, [3]Angus J Wilkinson

[1]*Department of Mechanical and Materials Engineering, Western University, Spencer Engineering Building, London, Ontario, Canada, N6A 5B9*

[2]*ESRF, 71 Avenue Des Martyrs, 38000 Grenoble, France*

[3]*Department of Materials, University of Oxford, Parks Road, Oxford, UK, OX1 3PH*

Abstract

The deformation of polycrystalline zirconium is analysed at the individual grain level using three-dimensional Synchrotron X-ray Diffraction (3D-XRD) in combination with a Crystal Plasticity Finite Element (CPFE) model. The effects of elastic strains and lattice rotations on the shape and position of diffracted peaks are studied in detail. For this purpose, the three dimensional measured microstructure of a commercially pure zirconium (CPZr) sample was imported into a crystal plasticity finite element (CPFE) model to simulate the deformation of measured grains. The calculated lattice rotations and strains of the selected most active grains were subsequently used to forward simulate diffracted peaks. The simulated peaks are then compared to the 3D-XRD measured ones. It is shown that although the sample was deformed to 1.2% strain, soft grains exhibit significant peak smearing. Peak broadening is mostly affected by the deformation induced lattice rotation and less affected by the elastic strains. Further, the comparison of CPFE modelling and 3D-XRD results confirms that prism and basal slip are the most active systems and pyramidal <c+a> is present but only slightly active. A method is developed to determine the activity of possible slip systems. As an example, by comparing the simulated and measured peak positions as well as the rotations of the most affected diffraction peaks, it is shown that pyramidal <a> slip system is not active significantly at room temperature.

Keywords: deformation mechanism, three dimensional synchrotron diffraction, crystal plasticity, finite element, hexagonal close packed, polycrystals

1. Introduction

The improvement of materials constitutive equations demands continued development of new experimental techniques which can provide the information required for validating or updating the models. From the materials deformation prospective, these experiments can be conducted at different length scales provided that the necessary data required for predicting material behaviour can be extracted. For instance, at nano and micro scales, cantilever beams or pillars can be used to characterize mechanical properties of engineering materials. These experiments are mainly conducted by milling micro-beams which will be deflected while the force-displacement curve is recorded [1–6]. The measured force-displacement curve and the orientation of the pillar can then be compared to a crystal plasticity or dislocation dynamic simulation to extract critical resolved shear stress (CRSS) values of each individual active system. For instance, by milling cantilever beams with particular orientations, Gong and Wilkinson have isolated each active slip system in CPZr micro-cantilevers and measured CRSS values accounting for size effects and used these CRSS values to predict bulk polycrstal deformation using CPFE [7]. Further, in a set of carefully designed experiments, the response of α and β titanium pillars to various applied strain rates and the interaction between the two phases of the composite pillar were studied by Zhang et al [8,9] and Jun et al [10,11].