

# Polycrystals: Microstructure and Effective Properties Workshop

Poster Titles and Abstracts – Monday 26 March 2018

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## Virtual instancing of 3D microstructures

Simon Wyatt, Yi Qiu and Ben Britton – Department of Materials, Imperial College London

Polycrystalline deformation is controlled by the ensemble of grains in an aggregate. There are many tools that enable accurate assessment of the surface change in deformation state, such as the high resolution electron backscatter diffraction (EBSD) technique which measures local variations in elastic strain and lattice curvature, and this information can be correlated with microstructural imaging using conventional EBSD. Unfortunately, we know that the response of polycrystalline aggregates is controlled not only by the surface microstructure, and the role of the subsurface may influence strain pattern and deformation, particularly in fatigue and failure. In this presentation, we will discuss a method to generate a 3D microstructure geometry that replicates a close geometric approximation of the surface microstructure with a statistically informed 3D subsurface microstructure, and its impact on the range of deformation states simulated using a plane stress based crystal plasticity simulation using a the Damask FFT solver."Variant coupling of martensite and bainite structures in steels

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## Non-divergent continuum description of the edge-dislocation core

Max Boleininger – Culham Centre for Fusion Energy

Conventional linear elasticity theory predicts the strain-fields at a dislocation core to diverge, growing to infinity. It is known from atomistic simulations that dislocation cores have a finite width. We present here an analytical solution to a generalised and parameter-free Peierls-Nabarro model of the edge-dislocation displacement fields which features a finite core width, as well as the correct isotropic elastic behaviour at large distances from the core. The strain fields are in agreement with atomistic simulations for the example of the tungsten  $1/2[111](1-21)$  edge-dislocation."

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## 3D Study of Deformation in Nano-indentation: Micro-Diffraction & Crystal Plasticity

Suchandrima Das – University of Oxford

We show the use of Nye's dislocation tensor for calculating the density of geometrically necessary dislocations (GND) in the study of plastically deformed materials. When estimating GND density there is a question concerning the optimisation technique used to solve the under-determined set of equations linking Nye's tensor and GND density. A systematic comparison of the densities obtained by two widely used techniques, L1 and L2 minimisation, shows that both methods yield remarkably similar total GND densities. Thus the mathematically simpler, L2, may be preferred over L1 except when information about the distribution of densities on specific slip systems is required. To illustrate this, we compare experimentally measured lattice distortions beneath nano-indents in pure tungsten, probed using 3D-resolved synchrotron X-ray micro-diffraction, with those predicted by 3D strain-gradient crystal plasticity finite element calculations. The results are in good agreement and show that the volumetric component of the elastic strain field has a surprisingly small effect on the determined Nye tensor. This is important for experimental techniques, such as micro-beam Laue measurements and HR-EBSD, where only the deviatoric strain component is measured."

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## Type I, II and III residual stress analysis in polycrystals using FIB-DIC

Alexander Korsunsky – MBLEM, University of Oxford

Residual stresses are a complex quantity that manifest themselves across a range of scales. Until recently there has been a disconnect between the theoretical description and the practical capability for residual stress evaluation. The recent advent of novel measurement techniques such as HR-EBSD and micro-beam Laue XRD have opened new opportunities. However, these methods are restricted to the analysis of highly crystalline samples. In contrast, the new micro-ring-core FIB-DIC method is capable of evaluating residual stress in amorphous and highly deformed samples. Results will be presented for the analysis of Type I-II-III residual stresses in Ti-6Al-4V bent beam samples using the combination of FIB-DIC and eigenstrain analysis."



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