ESRF	**Experiment title:** **OLIGOCRYSTAL DEFORMATION ANALYSIS: 3D grain and strain mapping and crystal plasticity modelling**	**Experiment number**: MA-26
Beamline: ID11	**Date of experiment**: from: 26/04/06 to: 03/05/06	**Date of report**: 1 Sep 2006
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Report:

Understanding the deformation processes occurring within (intra-granular) and between (inter-granular) grains of metallic alloys is important for improving our capabilities of processing, alloy formulation, engineering component design, and durability and reliability. To date most efforts have focused on the analysis of either polycrystals (treated essentially as consolidated powders), or single crystals and bi-crystals. Oligo-crystals lie between these two extremes, and correspond to the situation when a small, but significant number of crystals (say, 10 or 20) lie within the volume of interest (VoI). Often this corresponds to situations when, as a consequence of high stress concentration at notches or contacts, the integrity of the entire structure depends on the deformation response and integrity of this selected group of grains.

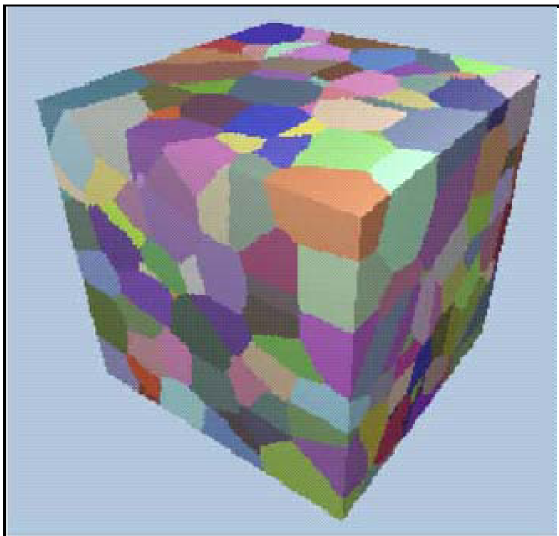


Fig.1. Grain orientation map illustration.

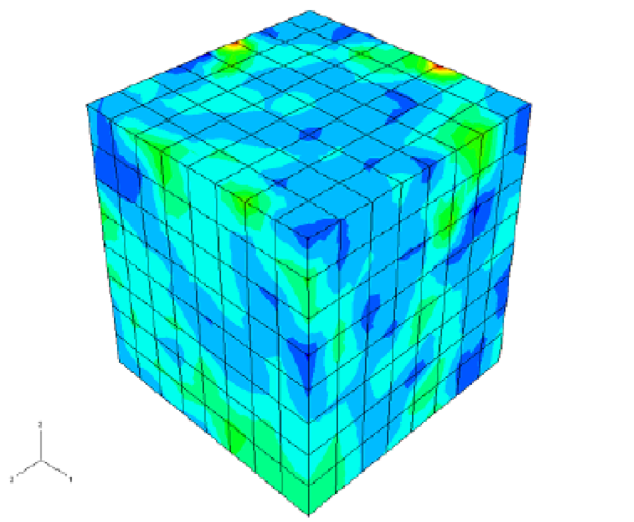


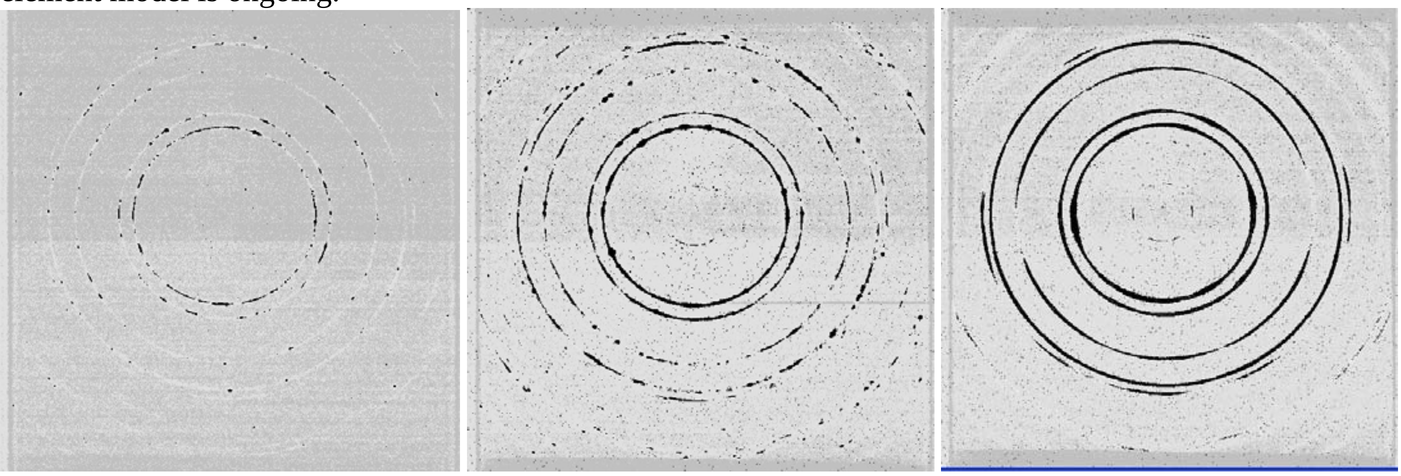
Fig.2. FE model strain map illustration.

We have built a 3D elastically anisotropic crystal plasticity finite element model capable of simulating the deformation of VoI's containing small numbers of grains. The model allows grain structure and orientation to be specified, and information relevant to the diffraction data to be extracted for the purposes of comparison and model validation. A crucial advantage of the FE model in question is that it captures the precise details of the relative grain positioning, thus offering an advantage over the mean field and self-consistent models. The model has already been validated against macroscopic deformation data and against polycrystalline

diffraction strain measurements. Oligocrystal diffraction data therefore is the most valuable and direct test of model's capability.

Aluminium alloy AA2124 samples were used as the principal material for investigation in this study. The specimen was prepared in the dog-bone shape with a 70mm gauge length, 6 mm width and 2 mm thickness. The 3DXRD microscope on ID11 was used to carry out pointwise mapping of grain orientation and strain. A rectangular three-dimensional array of 1000 points at 0.1mm spacing was interrogated within the specimen, filling a cubic volume of $1 \times 1 \times 1\ mm^3$. At each point within the matrix the sample needed to be rotated around a vertical axis in order to collect a redundant set of 2D oligocrystal diffraction patterns (the 'fan' set). The use of GraIndex post-processing routines then allowed us to extract all persistent grain orientations within the fan set. Since the volume at the fan apex remained within the beam in most cases within the fan set, it was possible to identify the crystal orientation that corresponded to this point within the array. The corresponding crystal strain was then ascribed to that point. The procedure for 3D orientation and strain mapping was quite laborious; however, it lends itself to routine treatment using suitably formulated selection algorithms. The situation may be compared to that encountered at the early stages of development of the EBSD (electron back-scattered diffraction) procedures that is now widely used for 2D (surface) mapping of micro-texture (but not strain).

The four-dimensional scanning carried out in the present experiment (mapping a 3D array of points with a 'fan' set collected at each location) required considerable time to complete. If the sample were maintained under load for the duration of the experiment, room temperature creep would be induced in the aluminium alloy sample. In order to overcome this problem, the 3D point array was first mapped in the sample prior to loading. The sample was then loaded to 6.2kN in tension, producing average macroscopic elongation strain 2% within the specimen. The specimen was then unloaded, and the 3D array set scanning was repeated. The purpose of this procedure is to allow the comparison to be made between orientation and strain distributions within the volume of interest pre- and post-deformation. The validation of the 3D finite element model is ongoing.



The final part of the experiment consisted of further *in situ* loading experimentas accompanied by strain measurement were carried out. These included rheo-diecast Mg alloy bar, high pressure diacast Mg alloy bar, IN 718 dog-bone specimen, and Ti-6Al-4V alloy dog-bone specimen. In situ loading and Debye-Scherrer geometry diffraction measurements were used to study the deformation, with the objectives to (i) incorporate elastic anisotropy into GSAS Rietveld refinement, (ii) add texture and twinning analysis to GSAS Rietveld refinement of deformed hcp structures, (iii) study of the relationship between single peak fitting and *a* and *c* lattice parameters obtained from Rietveld refinement of deformed hcp structures, (iv) identify bulk (average macroscopic) strain from diffraction data, (v) compare and contrast results from Ti and Mg alloys. The evolution of diffraction patterns with deformation (for nickel super-alloy IN718) is illustrated in the figure.

References

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