IITB-Monash Research Academy

Indian Institute of Technology Bombay | MONASH University

An Indian-Australian research partnership

Project Title:	**Microstructures in 4D. True representations of microstructural evolution**
Project Number:	**IMURA0248**

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Research Academy Themes:

Highlight which of the Academy's Theme(s) this project will address?

(Feel free to nominate more than one. For more information, see www.iitbmonash.org)

1. **Advanced computational engineering, simulation and manufacture**
2. Infrastructure Engineering
3. Clean Energy
4. Water
5. Nanotechnology
6. Biotechnology and Stem Cell Research

The research problem

Define the problem

The relationship between microstructure and materials properties is a basic tenet of materials science and engineering and yet there remains a gap in our ability to represent microstructure in unbiased descriptions of materials features. This gap is readily exposed when we try to predict or explain the properties of components in which there are few grains in the cross section: current models do not account for grain structures which have non-uniform distributions of shape and size, with variations in morphology and crystallography, and yet it is precisely these features which govern the performance of small components. In this project we will reconstruct the three-dimension microstructures of selected magnesium alloys by stereological deconvolution and serial sectioning. The project represents the state-of-the-art in using Dual-Beam FIB-SEM instruments to section a sample repeatedly with the ion beam and collect crystallographic orientation maps for each section using EBSD, allowing unsupervised segmentation of grains and grain boundaries. The FIB reconstruction would also be supplemented by mechanical polishing for serial sectioning.

Magnesium alloys are an attractive structural material due to its high strength to weight ratio. However, the hexagonal close pack (HCP) crystal structure of magnesium poses some unique challenges. The HCP structures do not have enough independent slip systems to accommodate plastic deformation in a polycrystalline system. Thus, twinning becomes a major mode of plastic deformation and a necessity. Moreover, the critical resolved shear stress for the basal slip system is orders of magnitude smaller that the other slips systems, thus the mechanical properties are highly anisotropic and the material can easily develop strong texture on deformation. Finally, since the twin behaves differently in tension and compression, the magnesium alloys show high degree of asymmetry.

The dominance of one deformation mechanism over the other (slip vs twinning) in Mg is known to be a function of temperature and load paths. However, data to ascertain the quantitative contribution of one over the other is not present. This is essentially due to two factors. The first being that twinning occurs on specific crystallographic planes and hence observations of 2D metallographic sections would not reveal the true number density of these. The second being that there exists a strong correlation in grain size and the propensity of twinning, but again as in the previous case the observations in 2D sections would not capture the true size of the grains and hence would bias the results. Similarly, during heat-treatment the microstructure evolution would be governed by the stored energy which has contributions from both slip and twinning. The understanding of these changes in microstructure is hindered by the limited 2D view of the sections. Hence, the main focus of this project is to develop a comprehensive framework to study the microstructure evolution of Mg alloys in 3D. This would be achieved by three parallel approaches. The first approach would use 2D metallographic sections to deconvolute 3D information using standard stereology. The second approach would use advance stereological tools in conjunction with disector observations to generate direct 3D microstructural information. And finally, the third approach would use serial sectioning to reconstruct complete 3D microstructure.

The majority of data would be generated using high resolution large area 2D EBSD scans at IITB and Monash electron microscopy laboratories. This 2D data would be deconvoluted to 3D by unbiassed techniques of standard stereology. However, topological data is not revealed on 2D sections and thus cannot be deconvoluted using standard stereology. For such a study advance stereological techniques (disector, selector and fractionator) would be used.

Some selected samples would be studied by full 3D microstructural reconstruction using serial sectioning Focussed Ion Beam (FIB) approaches. This would be supplemented by mechanical polishing serial sectioning. The use of 3D serial sectioning to generate quantitative descriptions of the 3D microstructure is a technology which is only about 5-8 years old and emerging, with no prior use in the context of microstructure evolution for Mg alloys during thermo-mechanical processing. Data would be manipulated using Paraview software and the Monash High Performance Computing facility. The EBSD data would be analysed using 3D EBSD analysis software and topology analysis program developed at IIT Bombay.

In the context of the proposed work, it is not only the 3D characterization of the microstructure for a given alloy that is important; a quantitative description of the evolution of the 3D microstructure with thermo-mechanical processing is also required. The exposure at different temperatures and times is of prime significance, leading to a description of the time evolution of the 3D microstructure, i.e. 4D characterisation.

Project aims

Define the aims of the project

The aim of the proposed work is to understand contribution of strain energy stored in slip and twinning for the 3D microstructural evolution subject to a specified thermo-mechanical history in Mg alloys.

Expected outcomes

Highlight the expected outcomes of the project

Mechanistic based understanding of the plastic deformation in this HCP structure and role of this in microstructure evolution. This will provide a scientific basis and original contribution in obtaining a process route for optimal microstructure. Moving away from empirical guesses to theoretical physics based approaches.

How will the project address the Goals of the above Themes?

Describe how the project will address the goals of one or more of the 6 Themes listed above.

This project is centred on the goal of cost-reduction through advanced computational methods and computer simulation. Without HPC the data processing and consequent understanding that is intended to result from this project would not possible.