Type of presentation: Poster

IT-16-P-1689 A new approach to determine excess free volume at high-angle grain boundaries – a proof of concept

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Grain boundaries (GBs) have a significant impact on the physical, especially mechanical properties of polycrystals. The GBs are typically characterized by structure units which are different compared to crystalline unit cells. It is assumed that grain boundary excess free volume plays an important role since it can be related to the grain boundary energy and has a significant influence on the transport and thermodynamic properties (diffusion/segregation). It has been reported that different GBs exhibit rather different excess free volumes, i.e. different specific mass densities from the crystalline bulk [1,2].
In this study we describe a new approach to determine the excess free volume from high-resolution transmission electron microscopy (HRTEM) images. For this purpose, an image analysis tool has been designed that allows determination of the local mass density from HRTEM images. Thereto the intensities of the GB regions have been compared with that of the grain interiors and the difference identified to be proportional to the density change, $\Delta\rho = (I - I_{gb})/I$, where I is the intensity of the grain interior and I_{gb} is the intensity of the GB.
In order to prove this concept, symmetrical tilt GBs with zone axes along the [100], [110] and [111] directions have been generated using molecular dynamics simulation (applying the LAMMPS software [3]) and subsequently taken as input for the simulation of HRTEM images using the Kirkland code [4,5]. The maximal density change of the GB has been estimated to be around -6% for the analyzed GBs. Calculations show that this approach works for pure samples with thicknesses up to 15 nm including aluminum oxide layers. The reliability of this approach is evaluated for different artificially chosen configurations including chains of vacancies and solute atoms.
Experimentally, well-defined aluminum bi-crystals have been investigated using aberration-corrected HRTEM. The results are discussed with respect to the relation between local structure, excess free volume and specific excess energy density.

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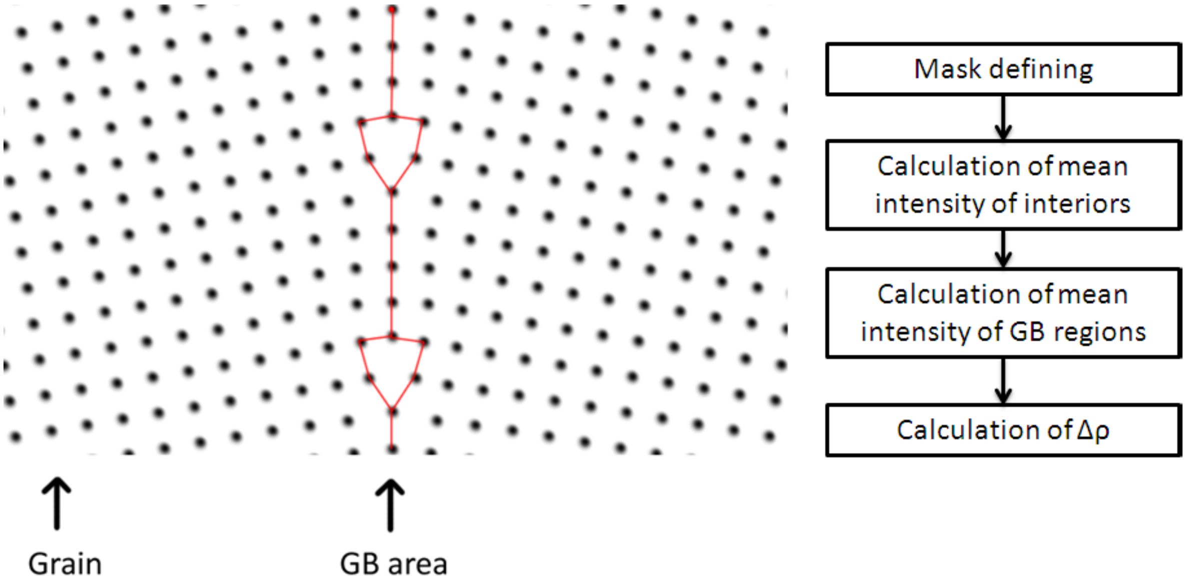

Fig. 1: Example of a symmetrical [100] tilt GB (left) and the work flow of the approach (right).

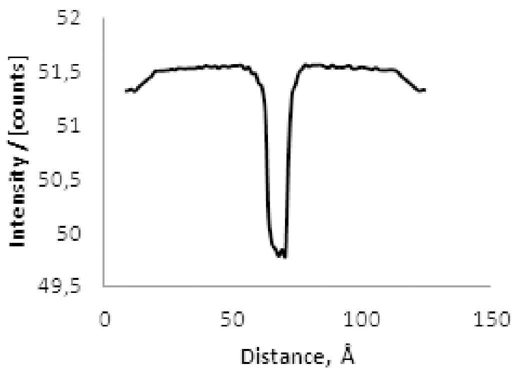

Fig. 2: Characteristic plot of the intensity across a symmetrical [100] tilt GB shown in Fig.1.

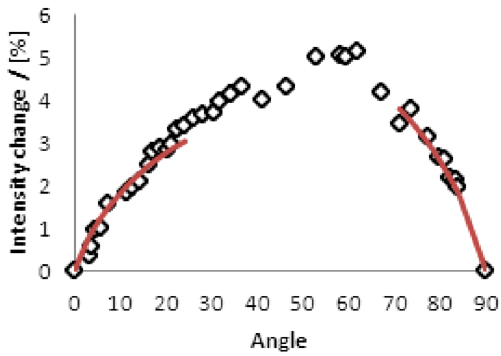

Fig. 3: Intensity change versus misorientation angle of simulated symmetrical [100] tilt GBs. Solid lines represent least squares fits to the data points.