Strain mapping of a Σ5(310) grain boundary in Cu bi-crystal using scanning transmission electron microscopy

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Background incl. aims
Grain boundaries (GBs) are pivotal in determining the physical characteristics of materials. The presence of extended strain fields localized at GBs can significantly impact atomic transport within these boundaries. Our research focuses on understanding the atomic structure of GBs and its correlation with the strain state along these boundaries. To delve deeper into the influence of strain on GB diffusion, we are investigating the evolution of strain along GBs under mechanical treatment using two distinct methods across varying length scales to establish a connection between microstructure and atomic transport properties.

Methods
A Cu bi-crystal containing a Σ5(310) GB was fabricated using a modified Bridgman technique, followed by annealing at 800 °C. An electron-transparent sample was prepared using FIB lamella target preparation to observe the GB in a cross-sectional view. The elastic strain along and across the GB was measured at the nanometer scale using a stack of nano-beam diffraction patterns (NBDPs) acquired in STEM mode with a 1 nm probe size, while ensuring grains were oriented in zone axis conditions. A custom-written code was utilized to extract the strain maps [1]. On an atomic scale, strain was characterized using the geometrical phase analysis (GPA) applied to high-resolution STEM images, based on measuring small displacements of lattice fringes relative to a reference lattice in the HR(S)TEM images [2].

Results
In the reference state of the pure Cu GB structure, shear strain, dilation, and rotation were measured along and across the GB using the NBDP method. The strain in the vicinity of the GB was found to be negligible (<0.1%). The results were consistent with the GPA method, showing almost constant small values of strain (<0.5%) in both halves of the crystal. These measurements were compared with strain mapping on cobalt-deposited samples.

Conclusion
Strain analysis of the GB in the Cu bi-crystal was conducted using two methods, GPA and NBDP, both of which yielded consistent results for strain across and along the Gb. GPA provided localized information at the nanometer scale, while NBDP offered strain information over a larger area. The strain analysis using GPA was correlated with the high-resolution structure of the GB. The high-resolution image of the GB provided insights into the variation of motifs within the boundary, potentially influencing strain distribution across both crystal halves.

Keywords:

Grain boundary, Strain, GPA, NBDP.

Reference:

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