Resolving grain boundary phase transformations in Copper by advanced STEM

Gerhard Dehm

Max-Planck-Institut für Eisenforschung, Düsseldorf;

Recently, it has been revealed by atomistic simulations that grain boundaries can undergo phase transformations leading to changes in material properties such as grain boundary diffusion. While faceting transitions of grain boundaries upon segregation had been reported earlier in literature, changes in the atomistic structure of grain boundaries as a function of chemical composition and/or temperature are experimentally largely unexplored. The excellent resolution of aberration corrected scanning transmission electron microscopy (STEM) provides direct access to the atomic structure of grain boundaries and their chemistry. In our studies we used bicrystals prepared in form of thin metallic films grown epitaxially on (0001) alpha Al_2O_3 substrates to study grain boundaries and their transitions in Cu. Bridgeman grown Cu bicrystals were alloyed with Ag to promote chemically driven grain boundary transitions.

In all cases grain boundary phase transitions or coexistence of two phase at the same grain boundary were observed. The structure motifs are discussed and compared to computational modelling. Strategies to determine experimentally whether grain boundary phases also impact material properties will be reported.

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