Revealing atomic motifs for grain boundary decoration in iron

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The atomic structure and composition of the grain boundaries have not been fully understood even for the simplest ∑5-grain boundaries. Several factors contribute to this difficulty: 1) representing the structure of grain boundaries requires more than five degrees of kinematic freedom; 2) the interplay between grain boundary structure and composition remains elusive, especially when it comes to imaging and quantifying light interstitial solutes, e.g. boron and carbon.

We have designed special sample geometries that restrict the kinematic freedom of the grain boundary, allowing for a systematic investigation of the relationship between structure and composition. Additionally, we have developed custom software to quantify the solute composition and distribution along the grain boundary planes using atom probe tomography (APT). This information is then correlated with the atomic structure obtained by state-of-the-art differential phase contrast (DPC)–four-dimensional scanning transmission electron microscopy (4DSTEM), which allows direct imaging of both the light solute atoms and the heavier iron atoms at the grain boundaries.

Our combined results demonstrate that even a change in the inclination of the grain boundary plane with identical misorientation impacts grain boundary composition and atomic arrangement. It is the smallest structural hierarchical level, the atomic motifs, that controls the most important chemical properties of the grain boundaries.

Acknowledgements: X.Z. acknowledges the support from Alexander von Humboldt Foundation (X.Z.). X.Z. acknowledge funding by the German Research Foundation (DFG) for funding via project HE 7225/11-1 (X.Z.). Work at the Molecular Foundry was supported by the Office of Science, Office of Basic Energy Sciences, of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231 (C.O.).