INTERDISCIPLINARY CENTRE FOR ADVANCED MATERIALS SIMULATION

ICAMS Seminar

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Cohesion at clean and doped grain boundaries in bcc Fe and Cr

The macroscopic strength of metal and alloys depends mainly on the cohesion at the boundaries of microscopic grains constituting the metal. Impurities segregated at the grain boundary (GB) can drastically modify its properties. The presence of impurities at GBs can lead to embrittlement (decohesion) or to strengthening of the material. Despite of several decades of research the mechanism of the embrittling/strengthening effect of various impurities is not well understood. Understanding cohesive properties of GB requires calculations in different scales starting from the quantum-mechanical scale. This talk discusses the effect of impurity atoms on the cohesive properties of GBs in bcc iron and chromium. The discussion is based on the results of calculations performed within the framework of density functional theory. Several different nonmagnetic (B, C, N, O, P, S) and magnetic (Cr) impurities at two different concentrations were considered in interstitial and substitutional positions at the symmetric GBs formed by the (210) and (111) surface tilts in ferromagnetic Fe. Also the effect of Fe impurity at the grain boundaries in antiferromagnetic chromium was considered. The changes in GB atomic geometries and energetics due to the modified electronic and magnetic structure caused by impurity atoms are presented and discussed. In particular, we discuss the embrittling/strengthening effect of the impurities and their segregation at the GBs. The latter is discussed in terms of chemical and mechanical components of the strengthening energy. In most considered cases, impurity atoms act as embrittlers to the Fe host structures. The magnetic properties of GBs are also discussed, in particular for the FeCr system.