Modélisation atomistique de la transformation de phase austénite-ferrite dans les aciers

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Abstract

This thesis applies the Quasiparticle Approach (QA) to investigate the atomic scale mechanisms driving the phase transformation from FCC to BCC structures in iron. Initially, the study focuses on pure iron, providing detailed results into the nature and role of dislocations, at the FCC-BCC interface. It was shown that the FCC-BCC interface is semi-coherent and stepped, with two sets of transformations dislocations at the interface. The QA framework reveals how each orientation relationship (OR) influences the interface characteristics. Although the ORs displayed different interface structures, all were ultimately found to follow the same atomic transformation path, driven by the glide of transformation dislocations at the interface. It was concluded that the complete FCC to BCC phase transformation involves the action of the Kurdjumov-Sachs (KS) transformation mechanism in two variants along the two sets of dislocations, with the Kurdjumov-Sachs-Nishiyama (KSN) mechanism emerging as the average of the two KS mechanisms. This detailed description served as a basis for the study of Fe-C systems, where carbon segregation at the interface was observed. Moreover, it was shown that the carbon concentration profiles were consistent with local equilibrium conditions at the interface