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ATOMISTIC SIMULATION OF CARBON SEGREGATION TO DISLOCATIONS IN ALPHA-IRON

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Abstract

The aim of this presentation is to present simulations of the formation of Cottrell atmospheres in iron with atomistic modelling. The goal is to capture the complex strain induced interaction between carbon and a dislocation. Molecular statics simulations with embedded atom method (EAM) potentials were carried out to obtain atomic configurations, carbon-dislocation binding energies, and the activation energies required for carbon hops in the neighborhood of the line defect. Simulations of the kinetics of carbon segregation towards the dislocation, in turn, were performed by means of a typical on-lattice Kinetic Monte Carlo (KMC) algorithm using information gathered from molecular statics. Results of this combined KMC-MD approach are in good agreement with thermoelectric power experiments performed on aged low alloyed steel.

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