

A story about iron and carbon: inputs from atomistic simulations

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An Fe-C inter-atomic potential has been designed to accurately describe the diffusion of C atoms in solid solution in alpha-iron (ferrite). This potential has been tested for many applications: the formation of a Cottrell Atmosphere (segregation of C to the dislocations core) observed during ageing, Zener ordering observed in fresh martensite. Recently, the potential has also been improved to describe the formation of carbides observed during martensite tempering.