Atomistic modeling of carbon diffusion in Fe-C martensite.

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Rapid quenching of austenite to room temperature often results in the formation of martensite phase. In the austenite the carbon atoms are randomly distributed on the octahedral sites of the face centered cubic (fcc) lattice and as usually after martensite transformation remains in the solid solution in this phase. Since only the z sites are common to both the fcc and bcc lattices, on transformation there are more carbon atoms at these sites causing the z-axis to expand. This why we can consider martensite as a supersaturated solid solution of carbon which has a body-centred tetragonal structure, a distorted form of bcc iron. Martensite phase is not stable at room temperature, and during aging decomposes into an inhomogeneous structure consisting of Fe and C rich nanodomains. This redistribution of carbon atoms involves the evolution of mechanical properties of martensite steels, this why the understanding of this phenomenon is quit important for applications.

In this work the atomistic modeling has been performed to investigate the transformation path kinetics in Fe-C system. It was shown that after Zener ordering the carbons atoms undergo the spinodal decomposition and form the carbon-rich nanodomains, which tend to align along <110> direction. Then some ordering structure appears following by the redistribution of carbon atoms through the three octahedral sublattices.

The microstructure of the carbon-rich phase is also analyzed by electron diffraction. It was shown that a modulated structure is formed, in which carbon-rich regions (precipitates) occur in a periodic manner throughout the sample, leading to the presence of diffuse streaks or satellite spots around each fundamental (matrix) reflection on the electron diffraction patterns. The simulated diffraction patterns are compared with experimental one and the evolution of tetragonality during aging is deduced. The simulated microstructure is also compared with atom probe images.