Atomic Density Function approach to model the carbon kinetics in martensite

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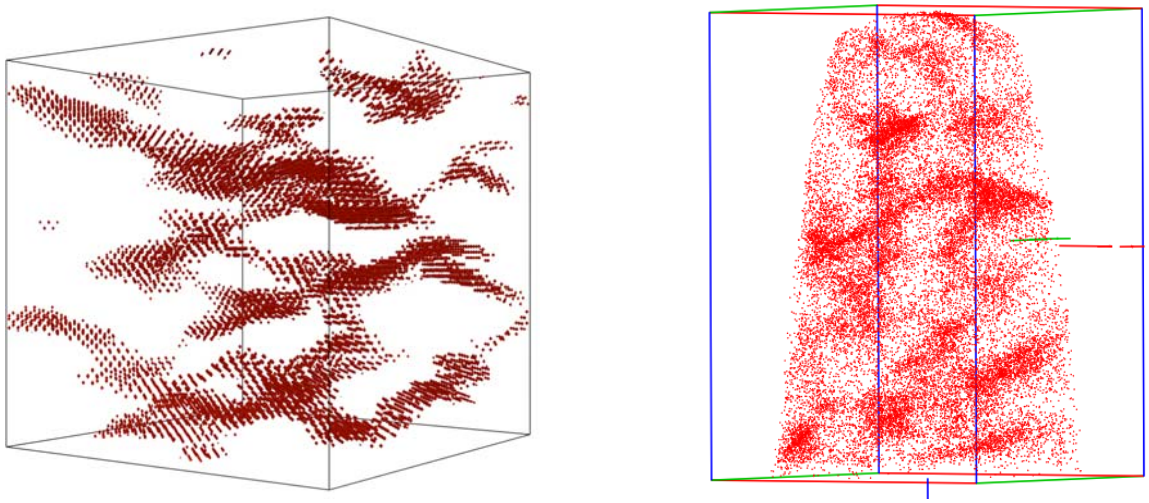
Carbon steels is the structural material by far the most used by man, and its importance in the global economy is paramount. This steel is Fe-C interstitial solid solution based on the low temperature bcc host lattice (α phase) and high temperature fcc solid solution (γ phase). Among its various forms, martensite obtained by rapid quenching the fcc austenite is the one with the highest strength. However, iron carbon martensite is not stable at room temperature and forms compositional modulations of carbon atoms during aging. It was shown experimentally that at the beginning these nanometric carbon-rich zones have Fe_8C composition and then undergoes C atom ordering within octahedral sublattices of the host Fe lattice. These carbon rich zones change drastically the mechanical properties of martensite. Consequently, it's extremely important to understand the phenomena related to low temperature (T<150°C) aging of the martensite in order to assist any further development of high strength steel.



a) b)

Figure 4: Redistribution of carbon atoms in the martensite aged 7 days at room temperature a) simulation results and b) 3D atom probe images. The carbon atoms are indicated in red.

In this study the Atomic Density Function (ADF) theory [1-4] has been applied to model the low temperature kinetics of carbon redistribution in martensite phase. It was shown that at early stage of aging the carbon kinetics is governed by the spinodal decomposition and small carbon rich zones appear. Then during further growth these zones are elongated to some special crystallographic directions to minimize the elastic energy of system. The simulated and experimental images of carbon redistribution in tempering martensite are shown in Figure 1. It should be noted that simulation results are in very good agreement with experimental data obtained by Atom Probe Tomography (APT).

References

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