Vacancy and self-interstitial assisted migration of Cr in FeCr alloys

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Solute transport due to vacancy migration is a mechanism that has been extensibly studied to reproduce the formation of precipitates in kinetic Monte Carlo algorithms (KMC). We recently published a model [1] for Object KMC algorithms featuring also the formation and migration of solute-vacancy pairs, so that the transport coefficients could also be reproduced [2] as well as the precipitates formation [3]. To complete the model for allowing point defects solute transport, as it occurs in irradiated materials, migration mechanisms of self-interstitials (SIA) including solute atoms (i.e. FeFe, FeCr, CrCr dumbbells) [4] have to be implemented along with the previous model. We present in this work out first results featuring SIA migration compared to previous calculations [2][5].

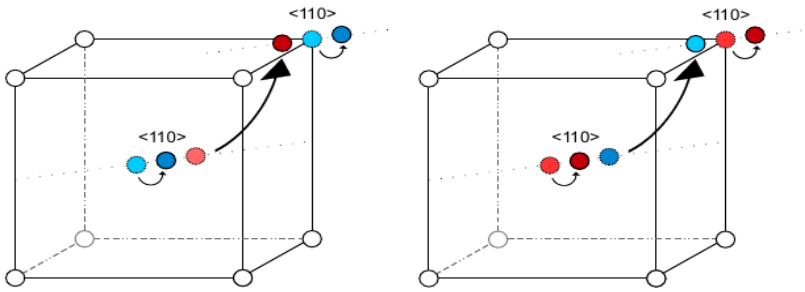

Figure 1: Some examples of migration mechanisms as implemented in the model. As there are 2 species and 3 implicated atoms (two from the initial dumbbell and the atom at the destination site) there are 8 cases.

References

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