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Multi-scale modelling of the structure and mobility of small defect clusters in iron MIHAI-COSMIN MARINICA, FRANCOIS WILLAIME, CEA, DEN, SRMP, F-91191 Gif-sur-Yvette — The mobilities of self-interstitial atoms (SIA) and their clusters in metals, especially body-centered cubic metals, are one of the main issues in multiscale models for the prediction of the microstructure evolution that these materials undergo under irradiation. In iron configurations made of non-parallel dumbbells and with a reduced mobility have been recently identified [1]. These results showed that non-conventional configurations and finite temperature effects must be taken into account [1]. We address these two points more thoroughly using on the one hand the activation relaxation technique [2], an eigenvector following method for systematic search of saddle points and transition pathways on a given potential energy surface, and on the other hand lattice dynamics calculations. For the most stable configurations, we have identified their migration mechanism. However, some clusters with low saddle point energies have to be considered in the kinetics of the system, although they are not linked to the most stable ones. Lattice dynamics free energy show that at high temperature configurations with <111> dumbbells and/or non-parallel dumbbells are favoured [1]. The low frequency modes at the origin of this are analyzed. 1. D.A Terentyev *et al*, Phys. Rev. Lett. 100 (2008)145503. 2. G.T. Barkema *et al*, Phys. Rev. Lett. 77 (1995) 4358; E. Cances *et al*, J. Chem. Phys. 130 (2009) 114711.

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