Determination of free energies of point defects by molecular dynamic simulation: Case of nickel.

EH. Megchiche[a] , H. Zenia[a] and K. Lounis[a]

[a] *Laboratoire de physique et chimie quantique, Université Mouloud Mammeri de Tizi-ouzou Tizi-ouzou, 15000,, Algeria, E–mail: megchiche@gmail.com*

At equilibrium all materials are characterized by presence of vacancies. Although the equilibrium concentration of vacancies is in general small, extra concentrations may be gen- erated by various processes when the material is acted upon by external agents, such as quenching, irradiation, oxidation, corrosion, and stress. Condensation and configuration of vacancy clusters play an important role in the evolution of damage in a variety of materials. In nickel experimental studies have shown the influence of point defects on the oxidation process. The hypothesis put forth by these experimenters to explain this phenomenon rests on an increased diffusion of oxygen inside the alloy, this being driven by a strong interaction between oxygen and vacancies. These are the vacancies present initially in the alloy, but also the ones injected at the metal-oxide interface during the oxidation process. Experimental characterization of point defects is often hindered by the limited resolution of the techniques in use, and also by the simultaneous presence of several kinds of defects in the system. Numerical simulations allow to isolate a defect of some kind and study it in detail. Therefore, simultation studies offer a valuable complement to experiments. However, so far finite temperature results are confined to those obtained using the quasi-harmonic approxi- mation, whose validity is limited to low temperatures. In this work we perform free energy calculations to study the stability of a divacancy in nickel at relatively high temperatures. We use well-tempered metadynamics with an embedded atom potential for direct free energy estimations. The main result is that the divacancy, while stable at low temperature, will dissociate at high enough temperature. The low temperature result is in agreement with the results obtained using the quasi-harmonic approximation. However, it is to be expected that the two methods will differ at high temperature.