

Multiscale modelling of the impact of hydrogen on mechanical properties of nickel base alloys

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The effect of hydrogen on plasticity remains unclear and it is revealed to be associated with phenomena which appear at different scales of the microstructure [1]. Hydrogen affects plastic flow behavior by acting on the short and long-range interactions of dislocations and vacancies. The aim of this work is to understand the mechanisms of hydrogen-microstructural defects interaction in nickel single crystal using nanoindentation and tensile simulations. Atomistic simulations of nanoindentation based on the Embedded-Atom Method (EAM) have been performed on nickel single crystals containing vacancies, with and without hydrogen. The effect of hydrogen on the pop-in load, softening effect in the elastic regime and hardening effect in the plastic domain have been questioned to define more relevant elementary processes. Based on these results, the hydrogen impact on apparent elasticity, activation volume and free energy in thermally activated forest interaction, cross-slip energy and length scales are implemented in dislocation-density based crystal plasticity model [2].

Keywords: nickel, hydrogen, plasticity, nano-indentation, atomistic simulations.

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