CAMT Seminar

“Development of interatomic potentials for modeling of hydrogen and carbon interaction near lattice defects in bcc iron”

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The introduction of hydrogen into metals and alloys leads to a variety of processes that make the materials more prone to failures. In high strength steels, the presence of hydrogen often embrittles the material by causing a sharp transition from ductile to brittle inter-granular fractures, accompanied by a drastic loss in toughness and ductility [1,2]. One of the reason for these hydrogen-mediated effects is the strong interaction between hydrogen impurities and other defects in the material such as vacancies [2,3], dislocation [4-6] and grain boundary. In order to advance the understanding about hydrogen related fractures of iron/steels, it is important to reveal the trapping states and distribution of hydrogen around various lattice defects and the effect of carbon on the interaction of hydrogen with defects. As the first step, within the atomic scale, we performed ab-initio simulations based on Density Functional Theory to investigate the stability and interactions of hydrogen and carbon around point defects in Fe-C-H systems. We found, among others, that as the number of trapped carbon increases, the accumulation of hydrogen around vacancy is reduced and vice versa. Furthermore, we extended the system to a much larger scale by developing interatomic potentials based on Embedded-Atom Method for the Fe-C-H ternary system to model non-equilibrium processes using Molecular Dynamics. The potentials was used for modeling the concentration of hydrogen and its interaction with carbon around symmetrical tilt grain boundary $\Sigma3\langle110\rangle\{112\}$. It is shown that, the concentration of hydrogen is high at low temperature and decreased when the temperature increases or there is presence of carbon impurities in the vicinity of the grain boundary.

References:

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