

Title: Ab-initio simulations of point defects and diffusion in cubic carbides

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Transition metal (TM) carbides with the cubic Halite structure, such as TiC and ZrC, combine ceramic-like properties with metal-like properties, which is a desirable combination for many existing and emerging applications of these compounds [1]. TiC and ZrC have great hardness at room temperature, but soften very rapidly with increasing temperature to become as soft as the respective metals already at about 1000 C. The softening effect can be remedied (or at least delayed) in a mixed carbide system (Ti,Zr)C, due to a spinodal decomposition into an ultrafine mixture of TiC- and ZrC-enriched regions. The decomposition is controlled by the rate of metal atom diffusion, and therefore the atomic mechanism(s) and other details of metal (Me) self-diffusion in cubic MeC compounds are of interest. This information is essential for modeling the structure and property evolution in hard materials during manufacturing and service. We employ ab initio calculations, using a plane-wave method [2] with projector augmented wave type pseudopotentials [3,4] and a gradient-corrected density functional [5], to systematically compute the energies and structures of point defects and their arrangements in MeC systems, as well as to simulate the processes of defect migration through the Halite lattice. Different mediators of Me diffusion have been considered previously, including clusters of vacancies [6,7] and interstitial atoms [8,9]. Here we revisit the diffusion mechanisms in MeC systems, based on the recent finding of a new (symmetry-broken) configuration of a Ti mono- vacancy in TiC that is almost twice lower in energy than the symmetric configuration. We explore the configurational space of a Me mono-vacancy to locate several energy minima. Among them, a planar symmetry-broken configuration with the optimal number, length, and angles of C—C bonds is found to be the global energy minimum. The formation of this and other symmetry-broken configurations is essential for describing Me self-diffusion in MeC by the mono-vacancy mechanism.

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Biography

Mehdi has completed his Msc in computational physics from the University of helsinki in 2016 and is currently a PhD student at KTH the Royal Institute of Technology in Stockholhm Sweden. His work is on Ab initio based multi-scale modelling of alloy phases and phase transformations. With a focus on multiscale computational models for studying materials, starting from the electronic and atomic structure of various defects (impurities, vacancies, stacking faults, dislocations, and grain boundaries) and extending to describe the interactions among these defects with the goal to predict the microstructure evolution and accompanying changes in the macroscopic mechanical properties of the material, taking into account external factors such as temperature and pressure.

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