POSTER REQUEST

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

M. Nourazar[1], E. Smirnova[3], P.A. Korzhavyi[1,2]

[1]KTH Royal Institute of Technology, Stockholm, Sweden
[2]Institute of Metal Physics, Ural Branch of RAS, Ekaterinburg, Russia
[3]NUST "MISIS", Moscow, Russia

E-mail: mehdin@kth.se

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.

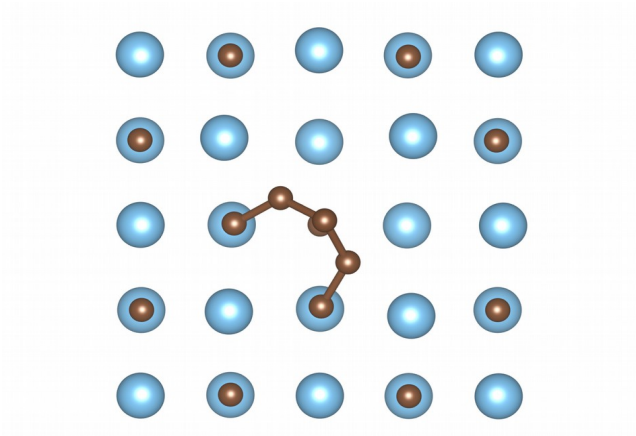


Figure 1: TiC "Horseshoe" open configuration with two Frenkel pairs.

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