

**FINDING POSSIBLE TRANSITION STATES OF DEFECTS IN SILICON-CARBIDE AND ALPHA-IRON USING THE DIMER METHOD** – F. Gao, W. J. Weber and L. R. Corrales (Pacific Northwest National Laboratory)\* G. Henkelman and H. Jónsson (University of Washington)

**EXTENDED ABSTRACT**

This is an extended abstract of a paper submitted for publication in the proceedings of the 6th COSIRES Conference, June 23-27, 2002, Dresden, Germany, to be published in Nucl. Inst. and Methods B.

The 'dimer' method was employed to search for possible transition states and their saddle point energies for interstitials and small interstitial clusters in SiC and  $\alpha$ -Fe. The dimer method is a technique for finding saddle points in the potential energy surface within a solid, without knowledge of the final state of transition, and without the use of second derivatives of the potential, has been recently developed by Henkelman and Jónsson [1]. In addition to the calculation of activation energies of point defect and cluster migration along the  $\langle 111 \rangle$  direction in  $\alpha$ -Fe, the activation energies for the directional change of interstitial clusters is investigated.

The dimer method, described in detail elsewhere [1], involves two atomic images of the system, separated by a very small 3N-dimensional unit vector. The energy of this dimer and the force on the midpoint, as well as the curvature of the potential at the dimer, can be calculated from the forces acting on the two images. The net force on the dimer is minimized by rotation of the dimer, and the dimer is translated so as to move up the potential surface. Saddle points are located through a series of rotations and translations of the dimer. Upon finding a saddle point, the dimer is returned to the starting configuration, and it is randomly assigned a new orientation as a starting configuration for another saddle point search. In principle, all saddle points surrounding the initial configuration can be found. In practice, the same saddle point or symmetrically equivalent saddle points are often found, and occasionally no saddle points are located after a reasonable expenditure of computer time. Once the saddle point is found, the minimum energy path to the next energy basin can be determined, and the changes in atom positions during the transition can be followed.

Silicon Carbide

The transition states and mechanisms for migration of interstitials in SiC are studied in a cubic box of 125 unit cells consisting of 1000 atoms with periodic boundary conditions. The lowest energy configuration for the C interstitial, based on the potentials used here, is the  $C^+C\langle 100 \rangle$  dumbbell at a C site, with a formation energy of 3.04 eV. This minimum state is used as the initial configuration for the saddle point searches. The dimer run consisted of 800 randomly chosen initial dimer orientations about this minimum. In SiC, the potential migration pathways for the C interstitial are found to consist of the first neighbor jump via a Si site, having an activation energy of 0.81 eV, or second neighbor jumps from a C site directly to another C site with activation energies on the order of 1.5 eV. The results for SiC are somewhat difficult to interpret, because the dimer method finds multiple shallow saddle points along a single transition path. The interatomic potential used for SiC in these calculations was developed by Gao and Weber [2] based on the Brenner formalism [3]. Tersoff potentials lead to similar behavior. Perhaps better potentials for SiC need to be developed.

Interstitials in  $\alpha$ -Fe

For interstitials and interstitial clusters in  $\alpha$ -Fe, supercells containing from 2000 to 8192 atoms are employed to ensure that the effects of interactions of a cluster with its periodic images are negligible. For single interstitials the  $\langle 110 \rangle$  dumbbell is used as an initial configuration for saddle point searches. Of 500 dimer searches, 425 converge to saddle points with an energy of 0.16 eV, which corresponds to the

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