SiC/SiC composites are one of candidates for the blanket structural material of future fusion reactors. The effect of irradiation on microstructure changes in the material has been recently reported in literatures, where voids are experimentally observed by TEM when irradiation temperature is greater than 1000 °C. This temperature is much greater than the corresponding temperature of void formation in metals during irradiation.

Nucleation and growth of defect clusters in materials during irradiation is determined by the net flux of mobile defects to the cluster. The outflux of mobile defects from the cluster is determined by the binding energy of mobile defects to the cluster. Unfortunately, however, such binding energy for silicon-carbide (β-SiC) is not clarified enough. In the present study, the binding energy of point defects to a vacancy cluster in β-SiC is investigated using a molecular dynamics (MD) technique. Interatomic potentials employed here for describing atomic interactions in β-SiC are the Gao-Weber potential. A crystal containing a vacancy cluster in β-SiC is first relaxed at finite temperature with an MD technique, followed by a quench to 0 K to obtain the total energy of the relaxed system. Subsequently, the formation energy of vacancy clusters and the binding energy of mobile defects to the cluster are obtained as a function of cluster size.

The calculated formation energy of isolated silicon and carbon vacancies in β-SiC is 3.49 eV and 2.56 eV, respectively. The formation energy of vacancy clusters shows an increasing function of cluster size, which is roughly in proportion to $n^{2/3}$, where $n$ is the total number of vacancies in the cluster. This size dependence is very similar to the case of voids in metals, although the formation energy of vacancy clusters in β-SiC is approximately 50 % greater than that of voids in bcc Fe. The binding energy of vacancies to a vacancy cluster in β-SiC is greater than that to a void in Fe, which may lead to the experimental fact of void formation at high temperature. Also, the binding energy of vacancies to a vacancy cluster depends on the constitution ratios of silicon and carbon vacancies contained in the cluster. With the binding energy thus obtained, the nucleation and growth process of voids in β-SiC is investigated using a kinetic Monte Carlo (KMC) technique.