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Point defects in cubic Boron Nitride(c-BN)

Thursday, 11 July 2019 15:00 (2 hours)

Point defects in cubic boron nitride are being investigated using the classical molecular dynamics and the rigid Tersoff potentials. In the process, the stability, the structural properties and lattice vacancies are being explored. The formulation uses the NVT Evans ensemble to obtain radial distribution functions and the defect energies for boron and nitrogen vacancies. Boron and nitrogen vacancy defect energies are calculated relative to bulk c-BN total energies. The results suggest that the nitrogen vacancy is more stable compared to the boron vacancy.

Apply to be
 considered for a student
   award (Yes / No)?

Yes

Level for award
 (Hons, MSc,
   PhD, N/A)?

Hons

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