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Stress-Defect Interactions at Molecular/Continuum Scales

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External stress on a crystal affects the Gibbs free energy of formation and migration of point defects, thereby lowering/raising defect concentrations and mobilities. This effect is determined by the volume change of the crystal-for defect creation it is the formation volume, Vt. Lattice distortion at the defect itself can only be predicted by atomistic simulations, not by continuum elasticity. However, this distortion, represented as a dipole tensor of forces in continuum elasticity, determines the far-field deformation, and hence Vt. For the vacancy in silicon, we have quantified Vt by such studies, using the Stillinger-Weber empirical potential at atomic scales and elasticity at continuum scales. We also have treated issues related to bridging these scales, obtained consistent interpretations of parameters, identified the limitations of continuum, molecular and ab initio calculations, and found overall agreement with relevant results by Eshelby.

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