THE CONTINUUM ELASTIC AND ATOMISTIC VIEWPOINTS OF FORMATION AND MIGRATION VOLUMES AND ENERGIES FOR SOLID STATE ATOMIC DIFFUSION

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We discuss the roles of continuum linear elasticity and atomistic calculations in determining the formation and migration volumes, and the strain energy of formation and migration of a point defect in a crystal. Our considerations bear special relevance to defect formation, and migration under stress, and therefore to atomic diffusion in the solid state. The elasticity treatment is based on the Green's function solution for a center of contraction or expansion in an anisotropic solid. It makes possible the precise definition of formation and migration volume tensors and leads to an extension of Eshelby's result for the work done by an external stress during the transformation of a continuum inclusion [1]. Parameters necessary for a complete continuum calculation of elastic fields around a point defect are obtained by comparing with an atomistic solution in the far field. However, an elasticity result makes it possible to test the validity of the formation/migration volume that is obtained via atomistic calculations under various boundary conditions. It also yields the correction term for formation/migration volume calculated under these boundary conditions. Using two types of boundary conditions commonly employed in atomistic calculations, a comparison is also made of the strain energies of formation and migration predicted by continuum elasticity and atomistic calculations. The limitations of the continuum linear elastic treatment are revealed by comparing with atomistic calculations of the formation and migration volume and strain energies of small crystals enclosing point defects. These findings have direct application to the formation and dissolution of nanostructures under stress.

References

[1] J.D. Eshelby "The determination of the elastic field of an ellipsoidal inclusion and related problems", *Proc. Roy. Soc. Lond. Ser. A,* ***241****(1226), 376, 1957.*

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