From coherent to incoherent mismatched interfaces: a generalized continuum formulation of surface stresses

Rémi Dingreville[1]

[1]*Sandia National Laboratories, Albuquerque, NM 87185 USA*
rdingre@sandia.gov

ABSTRACT

The equilibrium of coherent and incoherent mismatched interfaces is reformulated in the context of continuum mechanics based on the Gibbs dividing surface concept [1]. Two surface stresses are introduced: a coherent surface stress and an incoherent surface stress, as well as a transverse excess strain. The coherent surface stress and the transverse excess strain represent the thermodynamic driving forces of stretching the interface while the incoherent surface stress represents the driving force of stretching one crystal while holding the other fixed and thereby altering the structure of the interface. These three quantities fully characterize the elastic behavior of coherent and incoherent interfaces as a function of the in-plane strain, the transverse stress and the mismatch strain. The isotropic case is developed in detail and particular attention is paid to the case of interfacial thermo-elasticity. This exercise provides an insight on the physical significance of the interfacial elastic constants introduced in the formulation and illustrates the obvious coupling between the interface structure and its associated thermodynamics quantities. Finally, illustrations based on atomistic simulations of Cu [2, 3] and Cu/Cu2O interfaces [1] is given to demonstrate the relevance of the generalized interfacial formulation and to emphasize the dependence of the interfacial thermodynamic quantities on the incoherency strain with an actual material system.

References

[1] Dingreville R., A. Halli and S. Berbenni *From coherent to incoherent mismatched interfaces: A generalized continuum formulation of surface stresses*, Journal of the Mechanics and Physics of Solids, 72 pp. 40–60 (2014).

[2] Dingreville, R., and J. Qu., *Interfacial excess energy, excess stress and excess strain in elastic solids: planar interfaces.* Journal of the Mechanics and Physics of Solids, 56 (5) pp. 1944–1954 (2008).

[3] Dingreville, R., and J. Qu., *A semi-analytical method to estimate interface elastic properties.*Computational Materials Science, 46 (1) pp. 83–91 (2009).