Society of Engineering Science 51st Annual Technical Meeting 1–3 October 2014 Purdue University, West Lafayette, Indiana, USA

Twin boundary stability

Wright, Thomas, tim4906@comcast.net; Daphalapurkar, Nitin; Ramesh, KT, Johns Hopkins University, United States

ABSTRACT

Ideas from continuum mechanics are used to derive an elastic stability inequality for a contact plane between two different materials under quasi-static, homogeneous conditions. The terms in this inequality are interpreted for the case of an ideal twinning plane between two variants of a face-centered cubic material. High quality potentials for Ni and Cu are used in molecular dynamics calculations to calibrate relevant energies and displacements near the twinning plane. It is found that in comparison with direct molecular dynamics calculations the inequality predicts the critical stress in Ni within 1.9% and within 1.3% for Cu. Although the critical and calculated critical stresses are only upper bounds for the more realistic case of an imperfect boundary, the calculations give considerable insight into the interplay of energies that lead to boundary motion.