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A Generalized Approach for Solution to Image Stresses of Dislocations

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Abstract

This paper proposes an adaptive meshfree method to calculate the image stresses of the dislocations at the free boundaries and bicrystal interfaces. Based on the superposition method (van der Giessen and Alan Needleman, 1995) originally proposed for single crystal material with free boundaries, a weak formulation is developed for the bicrystal materials containing dislocations, where the interface constraints are imposed using Lagrangian multiplier. The meshfree approximation is introduced to improved the accuracy and smoothness from conventional FEM interpolation functions, and it is straightforward to adaptively enrich meshfree nodes at the surrounding area of dislocations to effectively improve the solution accuracy. The numerical examples demonstrate the effectiveness of the proposed method to calculate the image stress in 2D and 3D problems with various boundary and interface conditions using either the classical elasticity (J.P.Hirth and J.Lothe, 1982) or the singularity-free dislocation theory (M.Lazar, 2012, 2013, 2014; G.Po and M.Lazar, 2014).

Keywords: Dislocation dynamics, discrete dislocation, superposition method, image force, image stress, Element-free Galerkin, meshfree method

1. Introduction

Crystal defects in micro/nano-electronic-mechanical systems (MEMS/NEMS) such as semiconductor, in particular, dislocations, are very common in the device manufacturing process. The creation and motion of the dislocation affect not only the mechanical properties of the crystals, but also the device performance. For example, dislocations enhance junction leakage current which leads to degradation of the device performance. It is a critical issue in semiconductor industry to reduce process-induced dislocations(N.Tsuchiya, 2005). A typical kind of dislocations in the semiconductor is the misfit dislocation generated near the interface between the film and the substrate, which can be driven by the internal stresses due to the lattice mismatch. Although there are a number of theoretical(Frank FC, 1949a,b) and experimental (J.W.Matthews, 1961) study available, understanding dislocation behavior such as its mobility near the interface remains quite challenging.

The discrete dislocation dynamics (DDD) has a successful practice on studying dislocations in bulk crystals at submicron scales(L.P.Kubin, 1994; H.M.Zbib, 1999; N.M.Ghoniem, 2000;

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