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Mixed-mode singularity and temperature effects on dislocation nucleation in strained interconnects

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ABSTRACT

Dislocations can be nucleated from sharp geometric features in strained interconnects due to the thermal expansion coefficient mismatch, lattice mismatch, or stresses that arise during material processing. The asymptotic stress fields near the edge root can be described by mixed-mode singularities, which depend on the dihedral angle and material properties, and a transverse T-stress, which depends on how residual stress is realized in the interconnects. The critical condition for stress nucleation can be determined when an appropriate measure of the stress intensity factors (SIFs) reaches a critical value. This method, however, does not offer an explicit picture of the dislocation nucleation process so that it has difficulties in studying complicated structures, mode mixity effects, and more importantly the temperature effects. Using the Peierls concept, a dislocation can be described by a continuous slip field, and the dislocation nucleation occurs when the total potential energy reaches a stationary state. Through implementing this *ad hoc* interface model into a finite element framework, it is found that dislocation nucleation becomes more difficult with the increase of mode mixity, or the decrease of the T-stress, or the decrease of the length-to-height ratio of the surface pad, while the shape of the surface pad, being a square or a long line, plays a less important role. The Peierls dislocation model also allows us to determine the activation energy, which is the energy needed for the thermally activated, mechanically assisted dislocation nucleation when the applied load is lower than the athermal critical value. The calculated saddle point configuration agrees well with the molecular simulations in literature. Suggestions on making immortal strained interconnects are made.

1. Introduction

Interconnects in modern electronic applications usually consist of heterogeneous materials in layered and hierarchical structures (Hu, 1991; Freund and Suresh, 2004). Residual stresses are caused in materials that have different lattice constants or thermal expansion coefficients, or are intentionally or unintentionally introduced during the material processing (Kammler et al., 2005; Rudawski et al., 2009). For instance, the mobility of charge carriers in the integrated electronic structures, if strained, can be significantly enhanced. The great potential of the development of strained nano-electronics, however, is weakened by its susceptibility to dislocation injection, which can act as electrical leakage paths and fail the devices (Kammler et al., 2005; Zhang et al., 2006; Feron et al., 2007; Li et al., 2009). The critical condition for the dislocation injection near the stress concentration sites such as the edges or other geometric sharp features in these interconnected structures requires a knowledge of the dislocation nucleation process.

As a representative example in Fig. 1, a dislocation can be nucleated on the shaded plane from the edge of the film (or pad)-on-substrate system. The film or substrate may be stressed at faraway, or residual stresses arise from mismatches in lattice constants or thermal expansion coefficients. As will be shown in Section 2, regardless of how stresses are introduced in this structure, the stress fields near the edge root are singular and can be characterized by two parameters: the stress intensity factors (SIFs) and the transverse T-stress. Because of the asymptotic nature of the stress field, the linear elastic fracture mechanics shows that when an appropriate measure of the SIFs reaches a critical value, the dislocation will be nucleated (Zhang et al., 2006). This is essentially equivalent to the Rice–Thomson criterion, which states that a Volterra dislocation will be nucleated if the total driving force at a critical distance away from the stress singularity is larger than the lattice resistance (Rice and Thomson, 1974; Yu et al., 2007; Gao et al., 2008). However, the use of these phenomenological material parameters significantly limits the usefulness of the SIF-based method. Particularly we notice the following drawbacks:

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