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

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Article history:
Received 14 March 2010
Received in revised form 21 November 2010
Available online 7 January 2011

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.

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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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The SIF-based analysis does not provide a direct connection to the dislocation nucleation process. When the size of the dislocation nucleation process zone is comparable to the geometric feature or other length scales in the problem, the SIF-based method is clearly not applicable.

Interconnects involve complicated three-dimensional structures. It is difficult not only to characterize the three-dimensional asymptotic stress fields, but also to choose an appropriate measure of the critical SIF.

The stiffness mismatch of the film and substrate materials, as well as the dihedral angle at the edge root, will lead to a mixed-mode singular stress field (Hutchinson and Suo, 1992). Without an explicit treatment of the dislocation nucleation process zone, the relationship between the critical SIF and the degree of mode mixity cannot be determined.

Dislocation nucleation is a stress-assisted, thermally activated process. The temperature effects can be modeled by the calculation of the activation energy when the applied load is lower than the athermal critical value. The thermally activated dislocation will be a three-dimensional loop with a size depending on the degree of underload.

An explicit description of the dislocation nucleation process can be built up from the Peierls viewpoint, which models the dislocation core by a continuous distribution of the relative slip of two adjacent atomic layers lying immediately above and below the slip plane (Rice, 1992). The relative atomic slip field can be solved from the balance of the interface shear stress, the elastic interaction due to the applied stress (i.e., the SIF stress field), and the nonuniform slip distribution (i.e., the self-interaction of infinitesimal dislocations as determined from the slip gradient). Solving the resulting integral equations can be conducted by a numerical collocation method (Sun et al., 1993; Rice and Beltz, 1994), or by a variational boundary integral method (Xu et al., 1995; Xu and Zhang, 2003; Li and Xu, 2006; Segall et al., 2006), or by implementing such an ad hoc interface model into a finite element framework as shown in Section 3. The finite element approach has advantages in handling heterogeneous materials and complicated boundary conditions. The degree of mode mixity is determined and the critical stress for dislocation nucleation is calculated with respect to varying geometric and material properties. The Peierls framework also allows us to determine the activation energy, as presented in Section 4. It is found that the activation energy from the three-dimensional case is about 20\(b\) times of that from the two-dimensional calculations, where \(b\) is the magnitude of the Burgers vector. Results are compared favorably to the molecular simulations (Izumi and Yip, 2008), which are far more computationally expensive than our continuum model. In the concluding remarks in Section 5, we discuss how to design the interconnect patterns and materials to increase the critical stress for dislocation injection in the strained electronics.

2. Stress fields near the interface edge with respect to applied stress types

The source of residual stresses in the pad (or film)-on-substrate system (Fig. 1) can be external tractions, mismatch in thermal expansion coefficients or lattice constants, or resulted from the growth of materials, etc. If we apply a tensile stress in the x
direction, $\sigma_{xx,s}^{appl} (>0$, as in state A in Fig. 2), to a sufficiently thick and long substrate, the stress distribution for the state C in Fig. 2 (external stress applied on the film) can be determined from a linear superposition of A and B. In the stress state B, the applied stresses on the substrate and the film lead to the same strain in the $x$ direction, so that there is no shear stress on the interface. The applied stress on the film is thus given by

$$\sigma_{xx,f}^{appl} = \frac{E_f}{1-2\nu_f} \sigma_{xx,s}^{appl} = -\frac{1+\nu_r}{2} \sigma_{xx,s}^{appl},$$

where $E_f = E_f/(1-\nu_f^2)$, $E_s = E_s/(1-\nu_r^2)$, $E$ is the Young’s modulus, $\nu$ is Poisson’s ratio, respectively, and the subscripts “f” and “s” denote film and substrate, respectively. The parameter $\nu$ is one of the two Dandurs parameters:

$$\nu = \frac{\mu_s(1-\nu_r) - \mu_r(1-\nu_s)}{\mu_s(1-\nu_r) + \mu_r(1-\nu_s)}, \quad \beta = \frac{\mu_s(1-2\nu_s) - \mu_r(2-2\nu_r)}{2|\mu_s(1-\nu_r) + \mu_r(1-\nu_s)|},$$

which describe the stiffness mismatch of the two materials. Consequently, the stress states in A and C are related by

$$\begin{align*}
\sigma_{xx,f}^{th} &= \sigma_{xx,s}^{th} = \sigma_{C}^{th}, \\
\sigma_{xx,s}^{appl} &= \sigma_{C}^{appl}, \\
\sigma_{xy}^{th} &= \sigma_{xy}^{C}, \\
\sigma_{xx}^{appl} &= \sigma_{xx,s}^{appl} = \sigma_{C}^{appl}. \\
\end{align*}$$

The stress field can also be introduced by the thermal expansion coefficient mismatch (Timoshenko and Goodier, 1951). When the film-on-substrate system is stress free at a high temperature, $T_h$, the $x$-direction residual stress due to thermal expansion mismatch between the film and substrate after cooling to the room temperature $T_h$ can be written by the next equation under the plane strain condition:

$$\sigma_{xx,f}^{th} = \frac{E_f}{1-\nu_f^2} \left[ (1+\nu_r) \Delta x_f - (1+\nu_f) \Delta x_f \right]^T \Delta T,$$

where $\Delta T = T_h - T_0 < 0$. Note that this equation differs from the Stoney equation by the factor of $1+\nu$ in the braces, because the Stoney equation is derived for the biaxial stress field (Stoney, 1908; Freund and Suresh, 2004).

If $\sigma_{xx,s}^{th} = \frac{1+\nu_r}{2} \sigma_{xx,s}^{appl}$, the stress states in A and D are related by

$$\begin{align*}
\sigma_{xx,f}^{th} &= \sigma_{xx,f}^{D}, \\
\sigma_{xx,s}^{th} - \sigma_{xx,s}^{appl} &= \sigma_{xx,s}^{D} - \sigma_{xx,s}^{appl} = \sigma_{xx,s}^{D} - \sigma_{xx,s}^{th}, \\
\sigma_{yy}^{D} &= \sigma_{yy}^{D}, \\
\sigma_{zz,s}^{D} - \nu_r \frac{1+\nu_r}{2} \sigma_{xx,s}^{appl} - E_r \Delta x_f \Delta T &= \sigma_{zz,s}^{D} - \nu_r \frac{1+\nu_f}{2} \sigma_{xx,s}^{appl} - E_r \Delta x_f \Delta T = \sigma_{zz,s}^{D}, \\
\sigma_{yy}^{D} &= \sigma_{yy}^{D}, \\
\end{align*}$$

where $\sigma_{xx,s}^{th}$ is given in Eq. (4). It should be noted that $\sigma_{xx,f}^{D}$ and $\sigma_{xx,s}^{D}$ can be affected by thermal expansion coefficients. For instance, two cases (i) $(\Delta x_f, \Delta x_s, \Delta T) = (8 \times 10^{-6} \text{ K}^{-1}, 3 \times 10^{-6} \text{ K}^{-1}, 1000 \text{ K})$ and $(\Delta x_f, \Delta x_s, \Delta T) = (23 \times 10^{-6} \text{ K}^{-1}, 3 \times 10^{-6} \text{ K}^{-1}, 250 \text{ K})$ give the same $\Delta x_f \Delta T$ but different $\sigma_{xx,f}$ and Mises stress.

Yet another way of introducing stress is by predefining an initial stress field in the film, which can be realized in ABAQUS, a commercial finite element software (ABAQUS, 2008). The stress states in A and E are related by

$$\begin{align*}
\sigma_{xx,f}^{D} &= \sigma_{xx,f}^{E}, \\
\sigma_{xx,s}^{D} - \sigma_{xx,s}^{appl} &= \sigma_{xx,s}^{E} - \frac{1+\nu_r}{2} \sigma_{xx,s}^{appl} = \sigma_{xx,s}^{E}, \\
\end{align*}$$

Fig. 2. Schematic illustration of various stress states under plane strain condition.
The eigenvalues are denoted as the split singularity in literature (Liu et al., 1999; Zhang and Suo, 2007). The eigenvalue problem (Liu et al., 1999; Zhang and Suo, 2007), we have the same shear stress distribution at $r = 0$ as shown in Fig. 3. The last term in Eq. (8) is the T-stress (Rice, 1974; Tada et al., 2000). Solving the eigenvalue problem, the determinant of the coefficient matrix should vanish. In this paper, the singular stress field in the substrate around the root of the edge causes dislocation to be emitted, so that the associated coefficients are normalized by $\Sigma_{\text{ref}}(0) = 1$ as listed in Table 1.

Fig. 4 shows the distribution of radial stress $\sigma_r$ along the radial direction $r$ of the interface (thus $\sigma_{rr} = \sigma_{xx}$) for $\alpha = 0$, $L/H = 10$, $H = 100$ nm, and $\sigma_{\text{appl}} = 10$ MPa by using finite element simulations with a minimum element size of $e = 0.025$ nm. When the boundary condition of this eigenvalue problem, $\sigma_{\text{ref}} = \sigma_{\text{ref}}$ at $\theta = 0$, is considered.

Table 1

<table>
<thead>
<tr>
<th>$\alpha$</th>
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<th>0.5</th>
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<td>$\lambda_1$</td>
<td>0.4314</td>
<td>0.9130</td>
</tr>
<tr>
<td>$\lambda_2$</td>
<td>0.0915</td>
<td>0.9803</td>
</tr>
<tr>
<td>$\lambda_3$</td>
<td>0.4783</td>
<td>0.9795</td>
</tr>
<tr>
<td>$\lambda_4$</td>
<td>0.2542</td>
<td>0.4213</td>
</tr>
</tbody>
</table>

Fig. 3. Eigenvalues $\lambda_2$ as a function of the first Dundurs parameter $\alpha$ with the second Dundurs parameter being $\beta = 0$. The analytic solutions for this eigen-problem, the determinant of the coefficient matrix should vanish. In this paper, the singular stress field in the substrate around the root of the edge causes dislocation to be emitted, so that the associated coefficients are normalized by $\Sigma_{\text{ref}}(0) = 1$ as listed in Table 1.
ered, stresses obtained from the substrate and film elements should be identical, and the difference in numerical results would decrease with the decrease of element size. Using a very small element size and calculating \( k \) from Eq. (8) between \( 10^{-3} < r/H < 10^{-2} \), we confirm that the predicted stresses using \( k \) values fitted from the film stress agree with the finite element simulations as shown in Fig. 4. The substrate stresses for state D and E are lower than that of state A, which is due to the T-stress as shown in Eqs. (5) and (6).

The parameters \( k \) have different dimensions, and can be normalized by

\[
\begin{align*}
  k_1 &= \frac{S K k_1}{\mu b_s/\tau_{\text{max},s}}, \\
  k_2 &= \frac{S K k_2}{\mu b_s/\tau_{\text{max},s}} \\
  \eta &= \tan \psi = \frac{k_2}{k_1} A^{1/2},
\end{align*}
\]

Consequently, \( k_a \) can be normalized by

\[
\begin{align*}
  k_a &= \frac{r_{\text{res}a}}{H k_a} = \left( \frac{L}{H} \right) f_a \left( \frac{k_a}{\mu b_s/\tau_{\text{max},s}} \right)
\end{align*}
\]

Fig. 5 shows the distribution of normalized functions \( f_a \) as a function of \( \alpha \) and \( L/H \). The resulting mode mixture angle is shown in Fig. 6 with two choices of reference length, \( A = \mu b_s/\tau_{\text{max},s} \) or \( b_s \). It

![Fig. 5](image-url)

**Fig. 5.** Distribution of the normalized functions \( f_a \) with respect to \( L/H \) and \( \alpha \).

![Fig. 6](image-url)

**Fig. 6.** Mode-mixture angle \( \psi \) as a function of \( L/H \) for \( \alpha = -0.5, 0, 0.5 \) and \( H/b_s = 260 \) with two reference lengths: (a) \( A_1 = \mu b_s/\tau_{\text{max},s} \) and (b) \( A_2 = b_s \). These two length scales lead to \( \tan \psi_1 = \tan \psi_2 = (A_1/A_2)^{1/2} \).

![Fig. 7](image-url)

**Fig. 7.** Normalized critical stress, \( \sigma_{\text{crit}}/\tau_{\text{max},s} \) versus aspect ratio \( L/H \) for \( H/b_s = 260 \) and \( \tau_{\text{max},s} = 0.1 \). (a) \( \alpha = 0 \) with comparison of several stress states, and (b) \( \alpha = -0.5, 0, 0.5 \) for stress state A.
is found that with increasing α and decreasing L/H, the degree of mode mixity increases, and the degree of stress singularity decreases.

3. Dependence of dislocation nucleation condition on the mode mixity

Because of the asymptotic nature of the stress fields near the edge root, a dislocation will be nucleated if the magnitude of SIFs reaches a critical value, namely

$$S(\psi) = S_c(\psi),$$

(14)

where $S_c(\psi)$ can only be determined either by experimental measurements or by computation from a microscopic model. In the works of Feron et al. (2007) and Zhang and Suo (2007), the critical stress is calculated based on an assumption that dislocation is nucleated when the resolved shear stress reaches the theoretical shear strength $\tau_{\text{max},s}$ at a critical distance $r_c = b$. Consequently, we get

$$\sigma_{cL} = \frac{\tau_{\text{max},s}}{\mu_s} \left[ \left( \frac{H}{b} \right)^{\frac{1}{2}} F_1 \tau_{\text{max},s} \right],$$

(15)

where $n$ is the slip normal as shown in Fig. 1. Although the dependence on mode mixity is embedded in this equation, the choice of $b$ is questionable. For instance, the comparison between the Rice–Thomson model and atomistic simulations for dislocation nucleation from a surface step under compressive load suggests $r_c \sim 3 - 5b$ (Yu et al., 2007; Gao et al., 2008).

Li et al. (2009) have developed a method to simulate the process of dislocation nucleation from the edges/corners of a rectangular stress-free Si$_3$N$_4$ pad on a Si substrate via 3D finite element analysis using the Peierls dislocation model. The dislocation core is modeled by a continuous distribution of the relative slip of two adjacent atomic layers lying above and below the slip plane (Rice, 1992; Gao, 2010). The total energy will be increased by an interplanar potential, which is a periodic function of the relative atomic slip. The interface shear stress, being the spatial derivative of the interplanar potential, will restore the atoms to lattice registry and periodicity. The shear stress on the slipping interface $\tau_s$ is related to the relative slip $\delta$ by

$$\frac{\tau_s}{\tau_{\text{max},s}} = \sin \left( \frac{2\pi \delta}{b_s} \right) + \zeta \sin \left( \frac{\delta}{b_s} \right),$$

(16)

where $b_s$ is the magnitude of the Burgers vector of substrate and $\tau_{\text{max},s}$ is the maximum shear stress of substrate, i.e., the theoretical strength. Because the interplanar potential is periodic, a dislocation will be nucleated if the total potential energy reaches a stationary state.

It should be noted that a vast literature exists for the exact form of this interplanar potential, often called γ surface, which critically depends on atomic bonding, crystallographic orientations and shear directions, and tension-shear coupling, among many others (Rice, 1992; Xu et al., 1995). Because our objective in this paper is to examine the role of the geometric conditions and the resulting mode-mixity and T-stress, we merely adopt a simple sinusoidal form in Eq. (16), while the critical effects of the tension-shear coupling on the dislocation nucleation process (Sun et al., 1993; Xu et al., 1995; Xu and Zhang, 2003) are left for a future work.

Dislocation nucleation corresponds to an elastic snap-back instability that occurs after the total potential energy reaches an unstable equilibrium. In an implicit finite element formulation using Newton–Raphson iteration to solve the nonlinear equilibrium equations, one finds that the stiffness matrix becomes singular when the total potential energy reaches the stationary state. The numerical convergence difficulties immediately after the point of instability can be avoided by the introduction of the rate-depen-

dent dissipation term in Eq. (16). When $\zeta$ is chosen appropriately, the post-instability behavior can be accurately captured (Gao and Bower, 2004; Xia et al., 2007). This numerical technique is not meant to model any realistic energy dissipation mechanisms. Treating the interface as an ad hoc continuum, we have implemented Eq. (16) into the commercial finite element package, ABACUS, via a User-defined Element (UEL) subroutine. In two-dimensional calculations, this interface element is made of 4 nodes with 2 from each adjacent surface. As in a standard nonlinear finite element framework, given the displacement discontinuity field, the constitutive law specified in Eq. (16) is integrated to calculate the element stiffness, residual, and force vectors. Such a method can explicitly describe the dislocation nucleation process, whereas the SIF-based method (Feron et al., 2007; Zhang, 2007), being equivalent to the Rice–Thomson criterion (1974), does not provide an explicit treatment of dislocation nucleation process.

In the results presented in Figs. 7–10, the interface elements are inserted along the slip plane as shown in Fig. 1(b). The critical stress for problem A, or D, or E is the stress, $\sigma_{\text{cr},l}/\sigma_{\text{cr},s}$, or $\sigma_{\text{cr},l}/\sigma_{\text{cr},s}$, respectively, when dislocation nucleation occurs. These choices ensure that the comparison is made for the residual stress in the film. Fig. 7(a) shows the critical stress for dislocation nucleation as a function of aspect ratio $L/H$ with $b = 0.383$ nm, $\tau_{\text{max},s}/\mu_s = 0.1$, $H = 100$ nm, and thermal expansion coefficients of $\gamma_f = 11 \times 10^{-6}$ K$^{-1}$ and $\alpha_s = 3 \times 10^{-6}$ K$^{-1}$ (for state D only). As the $L/H$ ratio decreases, the critical stress increases, because the stress

Fig. 8. Normalized critical stress $\sigma_{\text{cr},l}/\tau_{\text{max},s}$ versus aspect ratio $L/H$ of Si$_3$N$_4$ pad with $H/b_s = 260$. (a) $\tau_{\text{max},s}/\mu_s = 0.2$ and (b) $\tau_{\text{max},s}/\mu_s = 0.1$. Note that the results based on the stress intensity factors are the same in these two cases.
concentration decreases as the two side surfaces (i.e., \(yz\) planes) move together (Feron et al., 2007; Li et al., 2009). The stress fields in states D and E are the same except for the \(zz\) component, which does not affect dislocation nucleation process for the slip system considered in Fig. 1. The stress fields in state A differs from those in D and E in the T-stress, as shown in Eqs. (5) and (6). The critical stress for state D can be derived from that for state A, and vice versa, from the following procedure. If the maximum resolved shear stress in state D, as given by

\[
\sigma_{\text{crit}}^{\text{A}} / \sigma_{\max,s} = \frac{1 + \alpha}{1 - \alpha} \left( \frac{\tau_{\max,s}}{\sigma_{\text{crit}}^{\text{A}} (1 - \alpha)} - \cos \varphi \sin \varphi \right),
\]

(17)

The critical stresses obtained from the above model are different only within 5% from the finite element results in Fig. 7(a). Therefore, we can conclude that the difference of the critical stresses among various stress states in Fig. 2 is caused by the T-stress projected on the slip system.

The effect of Dundurs parameter \(\alpha\) on the critical stress for state A is shown in Fig. 7(b). The critical stress increases with \(\alpha\) value, since when the substrate properties are fixed, an increase of \(\alpha\) leads to a decrease of the residual stress in the substrate. For example,

\[
\sigma_{\text{crit}}^{\text{A}} / \sigma_{\max,s} = 3 \text{ GPa in the substrate when } \alpha = 0 \text{ and } \sigma_{\text{crit}}^{\text{A}} = 3 \text{ GPa in the film, whereas } \sigma_{\max,s} = 1 \text{ GPa in the substrate when } \alpha = 0.5 \text{ and } \sigma_{\text{crit}}^{\text{A}} = 3 \text{ GPa in the film. Hence, as } \alpha \text{ increases, the stress concentration at substrate decreases and therefore the critical stress increases.}
\]

We also consider the example of a silicon nitride (\(Si_3N_4\)) pad on a silicon (\(Si\)) substrate. Following Feron et al. (2007) and Zhang and Suo (2007), we take the shear modulus and Poisson’s ratios of \(Si_3N_4\) to be 54.3 GPa and 0.27 and those of silicon to be 68.1 GPa and 0.22, respectively. The corresponding exponents \(\lambda_e\) and coefficients of function \(\Sigma_2(\psi)\) are given in Table 2. As shown in Fig. 8, the three curves show a similar trend with respect to \(L/H\), but the differences are quite dramatic. It should be noted that the model in Eq. (15) predicts a proportional relationship between \(\sigma_{\text{crit}}^{\text{A}}\) and \(\tau_{\max,s}\), i.e., re-

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**Table 2**

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</tr>
<tr>
<td>0.1411</td>
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**Fig. 9.** Normalized critical stress \(\sigma_{\text{crit}}^{\text{A}} / \sigma_{\max,s}\) versus normalized length scale \(\tau_{\max,s} / \mu b_s\) of \(Si_3N_4\) pad for \(L/H = 2\) and 10.

**Fig. 10.** Normalized critical stress \(\sigma_{\text{crit}}^{\text{A}} / \sigma_{\max,s}\) versus mode-mixity angle \(\psi\) for various \(L/H\) ratios and \(\alpha\) values (0.5, 0, and 0.5) with reference lengths \(\Lambda = \mu b / \tau_{\max,s}\).
results denoted by filled circles in Fig. 8(a) and (b) are identical. But our Peierls-type model shows a dependence on \( \tau_{\text{max,sl}} / \mu_c \). Results for different \( \tau_{\text{max,sl}} / \mu_c \) ratio can be normalized and collapsed onto master curves in Fig. 9. The ratio, \( \sigma_{crl} / \tau_{\text{max,sl}} \), depends only on \( \tau_{\text{max,sl}} / \mu_c \), aspect ratio \( L/H \), and Dundurs parameters. These results also suggest that a better choice for the critical distance used in Eq. (15) be \( \mu_c b / \tau_{\text{max,sl}} \), which scales as the dislocation core size.

The relationship between the critical stress and mode-mixity angle is obtained by compiling data in Fig. 6(a) and Fig. 7(b) and performing similar calculations for \( \tau_{\text{max,sl}} / \mu_c b_c = 10 \), as shown in Fig. 10. The mode-mixity angle only varies in a small range in this study with respect to varying \( L/H \) and \( \delta \). The critical stress increases with the mode-mixity angle \( \psi \), and a small change of \( \psi \) may lead to several times of change in \( \sigma_{\text{crl}} \).

4. Dependence of dislocation nucleation condition on temperature

The critical stress calculated in Section 3 is the athermal critical value, i.e., the stress needed for dislocation nucleation at zero temperature. When the applied stress is lower than this athermal limit, the thermal energy can be large enough to overcome an energy barrier for the dislocation nucleation to occur (Rice, 1992; Bei et al., 2008; Gao, 2010). Such an energy barrier increases as the increase of the underload (i.e., the athermal limit minus the residual stress in film). The activation energy for the dislocation nucleation from a crack tip has been studied using the Peierls framework (Rice and Beltz, 1994; Xu et al., 1995). In these calculations, a slanted interface model has been suggested (Rice, 1992) which excludes the elastic displacement caused by periodic shear stress along the slip plane. The resulting constitutive relationship in the interface model is defined by

\[
\frac{\tau}{\tau_{\text{max,sl}}} = \sin \left( \frac{2\pi \Lambda}{b} \right), \quad \delta = \Lambda - \frac{b}{2\pi} \sin \left( \frac{2\pi \Lambda}{b} \right),
\]

\[
\Phi(\delta) = \frac{\tau_{\text{max,sl}} b}{\pi} \sin^2 \left( \frac{\pi \Lambda}{b} \right),
\]

where \( \Phi \) is the interface potential energy per unit area. Whether using the sinusoidal model in Eq. (16) or the slanted model in Eq. (18) gives a negligible difference in the calculation of the athermal strength (below 1% difference in our finite element simulations), but the activation energy calculations can be drastically different (Rice and Beltz, 1994).

To determine the activation energy for dislocation nucleation in the film-on-substrate system under a given applied stress, \( \sigma_{\text{appl}}^{\text{sl}} < (1 - \alpha) \sigma_{\text{crl}}^{\text{sl}} / (1 + \alpha) \), we need to find the stable equilibrium solution, \( \delta_{\text{min}}(x) \), and the saddle-point configuration, \( \delta_{\text{sad}}(x) \). The activation energy is thus given by

\[
\Delta U_{\text{act}} = U[\delta_{\text{sad}}(x)] - U[\delta_{\text{min}}(x)].
\]

Fig. 12. Normalized activation energy \( (1 - \psi) \Delta U_{\text{act}} / \mu_c b^2 \) versus applied stress \( \sigma_{\text{appl}}^{\text{sl}} \) as normalized by (a) \( \tau_{\text{max,sl}} \) and (b) \( \sigma_{\text{crl}}^{\text{sl}} \), respectively. Other parameters include \( \alpha = 0 \) and \( \tau_{\text{max,sl}} / \mu_c = 0.1 \).

Fig. 13. Saddle-point configuration at \( \sigma_{\text{crl}}^{\text{sl}} / \tau_{\text{max,sl}} = 0.54 \). Other parameters include \( H/b_c = 260, L/H = 2 \), and \( \tau_{\text{max,sl}} / \mu_c = 0.1 \). (Note that \( \sigma_{\text{crl}}^{\text{sl}} / \tau_{\text{max,sl}} = 0.768. \)  

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**Fig. 11.** Displacement profiles for various \( x \)-directional applied stresses on substrate for \( x = 0, L/H = 10, H/b_c = 260 \), and \( \tau_{\text{max,sl}} / \mu_c = 0.1 \).
where under two-dimensional condition
\[
U^{2D}[\delta(x)] = U_0 + \int_0^\infty \Phi[\delta(x)]dx - \frac{1}{2} \int_0^\infty \frac{\tau_{\text{elas}}(x)}{C_1} dx.
\]  
(20)

The first term in Eq. (20) is the potential energy of the elastic system when the interface slip is zero, the second term gives \( \Phi[\delta(x)] = \Phi(\delta(x)) - \frac{1}{2} \delta(x) \Phi'(\delta(x)) \), and the third term integrate the product of interface slip and the elastic shear stress field, \( \tau_{\text{elas}}(x) \), when the interface slip is zero. Three set of finite element simulations are therefore required to calculate Eq. (20). We first perform elastic analysis to determine \( \tau_{\text{elas}} \) from the stress components by the Schmid law, \( \tau_{\text{elas}} = m \sigma_{ij} b j / b \). The stable equilibrium can be calculated by smoothly increasing the applied load from the initial condition \( \delta(x) = 0 \). To obtain the saddle-point configuration, an initial slip field is imposed on the interface nodes along the slip plane in step one. Then the remote \( x \)-direction load is gradually increased up to the desired load level on the outside surface of the substrate in step two. The fictitious viscosity method in Eq. (16) is not needed in such calculations. A typical result for stress state A is shown in Fig. 11 with \( L/H = 0.1 \), \( \alpha = 0 \), and \( \tau_{\text{max},s}/\mu_{b} = 0.1 \). The slip distributions for representative load values are similar to those obtained from 2D analysis of dislocation nucleation from a mode-II crack tip (Rice and Beltz, 1994). However, when \( \sigma_{xx, s}/\tau_{\text{max},s} = 1 \), the maximum slip does

![Diagram](image)

**Fig. 14.** Saddle-point configuration at load level: (a) \( \sigma_{xx, s}/\tau_{\text{max},s} = 0.58 \), and (b) \( \sigma_{xx, s}/\tau_{\text{max},s} = 0.70 \). The interface slip along the \( r \) direction is plotted in contours. Other parameters include \( H/b_s = 260 \), \( L/H = 2 \), and \( \tau_{\text{max},s}/\mu_{b} = 0.1 \).

![Diagram](image)

**Fig. 15.** Normalized 3D activation energy \( (1 - \nu) \Delta U_{\text{act}}^{3D}/\mu_{b}^3 \) with respect to the normalized applied stress \( \sigma_{xx, s}/\tau_{\text{max},s} \) for (a) \( L/H = 2 \) and (b) \( L/H = 10 \). Comparisons to literature work are shown in (c).
not reach \( b_1/2 \) at the crack tip, which is a consequence of the mixed-mode singularities.

The activation energies are calculated at various stress levels and geometries. As shown in Fig. 12, for a given set of \( r_{\text{max},d}/\mu b \) and \( z \), when \( L/H \) or \( H/b \) decreases, larger activation energy is needed at a given applied stress, because the critical stress is inversely proportional to \( L/H \) as shown in Fig. 9. However, when the applied stress \( \sigma_{\text{cr}}^{\text{appl}} \) is normalized by the corresponding critical stress \( \sigma_{\text{cr}}^{\text{cr}} \), the activation energy function is insensitive to the variation of geometry as shown in Fig. 12(b).

In the two-dimensional analysis, saddle point configurations calculated in Fig. 11 do not depend on the \( z \) coordinate. This kinematic constraint can be relieved in the three-dimensional simulations. As shown in Fig. 13, both eight-node hexahedral elements (C3D8) and user-defined interface elements are used, and a half model in \( z \) direction is used because of symmetry. The calculation cell size in the \( z \) direction is about \( 30b \). The entire finite element model consists of about 106,400 elements and 116,900 nodes. The minimum element sizes along both \( x \) and \( y \) directions are the same as those in the 2D case, and the element size in the \( z \) direction is chosen very large when moving far away from the symmetric plane. The activation energy calculation is similar to Eq. (20), except that the slip distribution is \( \delta(r,z) \) and a double integral \( \int_0^{\infty} \int_0^{\infty} \delta(r,z) \, dr \, dz \) should be adopted, where \( r \) is the radial coordinate along the slip direction.

The saddle point configuration resembles a half elliptical dislocation loop, as shown by the displacement plot for \( \sim 30\% \) underload in Fig. 13, and the slip contours of \( \delta_r \) for \( \sim 30\% \) underload in Fig. 14(a) and for \( \sim 10\% \) underload in Fig. 14(b). A summary of 2D and 3D results is given in Fig. 15, which suggests that the 3D activation energy (unit: Joule/meter) is roughly equal to the product of 2D activation energy (unit: Joule/meter) and 20b. Again, when normalizing \( \sigma_{\text{cr}}^{\text{appl}} \) by the athermal strength, the activation energy curves are not sensitive to the geometric parameter \( L/H \) as shown in Fig. 15(c).

Our Peierls-type model agrees with molecular simulations by Izumi and Yip (2008), who considered the dislocation nucleation in a sharp edge in Si. Their activation energy curves, as well as a Rice–Thomson-type analysis, are also plotted in Fig. 15(c). Rice and Beltz (1994) suggest that for the thermally activation dislocation nucleation to occur, the activation energy should be \( \Delta U_{\text{act}}^{\text{3D}} < 30 k_B T \), where \( k_B \) is the Boltzmann constant. This corresponds roughly to \( (1 - v_1) \Delta U_{\text{act}}^{\text{2D}} / \mu b^4 \lesssim 0.1 \) for Si and \( T = 1000 \, \text{K} \). A 15% underload at this temperature may still lead to thermal nucleation by Izumi and Yip (2008), but our results predict a borderline of 5% underload. One reason for this discrepancy is that their molecular simulation studies considered a hexagonal slip plane, and the calculated saddle point configuration resembled a polygon rather than an ellipse in our results. In addition, the interplanar potential used in Eqs. (16) and (18) may be dependent on the distance between the interface element and the free surface, because surface atoms are in a different bonding environment from those in the bulk (Zhu et al. (2008)).

The three-dimensional characteristics of the nucleated dislocation can result from thermal activation as well as from the nonuniform stress field. Results in Fig. 16 for a square Si\(_3\)N\(_4\) pad on a Si substrate were adapted from our previous work (Li et al., 2009). The first dislocation is nucleated from the corner of the surface pad, whereas the second one from the center of the surface pad because the stress fields near the edge root have been changed due to the back stress of the first dislocation. Therefore the stress nonuniformity due to complex interconnect patterns, as well as the thermally activation dislocation loops, may lead to a three-dimensional dislocation microstructure near the sharp geometric features.

5. Concluding remarks

Dislocation emission from sharp geometric features in strained interconnects critically depends on mixed-mode singularity, T-stress, slip systems, aspect ratio and shape of the interconnect patterns, and temperature. A method to calculate the critical condition for dislocation nucleation and the activation energy has been developed by using finite element analysis based on the Peierls-type dislocation model. This method offers an explicit description of the dislocation nucleation process, and is thus more rigorous than the SIF-based analysis. This continuum model can conveniently determine the activation energy, and is much less computationally demanding than molecular simulations.

Fig. 16. Dislocation loops nucleated from a square Si\(_3\)N\(_4\) pad on the Si substrate. Because of symmetry, a half model in \( z \) direction is used. Parameters used include \( H/b_1 = 20 \), \( r_{\text{max},d}/\mu = 0.21 \), and \( L/H = 10 \).
Insights on making immortal, strained nano-electronics can be obtained from our analyses. It is shown that the increase of mode mixity, which can be achieved by choosing different material combinations, or the decrease of T-stress, which can be achieved by varying boundary conditions, can increase the critical stress for dislocation injection. Throughout this paper, we assume that the slip plane intersect with the edge root, while dislocation nucleation in an inclined slip plane is more difficult. Consequently, when the stress is intentionally introduced in the substrate to enhance functional performance, the most effective way to avoid dislocation nucleation is to vary the crystallographic orientations. In our previous study (Li et al., 2009), we have shown that the decrease of L/H will increase the critical stress for dislocation nucleation, while the shape of the surface pad (i.e., being a square or a long line) plays a negligible role. There, however, exists a possibility that changing the shape and pattern of interconnects can change the T-stress.

Acknowledgements

Financial support for this work was provided by the National Science Foundation (CMII 0800168 and CMMI 0900027), and the Center for Materials Processing at the University of Tennessee. J.H.L. was partially supported by the Korea Research Foundation Grant (Grant No. KRF-352-D00001) funded by the Korean Government (MOEHRD). Research at the Oak Ridge National Laboratory was sponsored by the Division of Materials Sciences and Engineering, Office of Basic Energy Sciences, U.S. Department of Energy, under contract DE-AC05–00OR22725 with UT-Battelle, LLC.

References