Split singularities and dislocation injection in strained silicon

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Abstract

The mobility of charge carriers in silicon can be significantly increased when silicon is subject to a field of strain. In a microelectronic device, however, the strain field may be intensified at a sharp feature, such as an edge or a corner, injecting dislocations into silicon and ultimately failing the device. The strain field at an edge is singular, and is often a linear superposition of two modes of different exponents.

The relative contribution of the two modes is characterized by a mode angle, and the critical slip systems are determined as the amplitude of the load increases. Critical residual stress is calculated in a thin-film stripe bonded on a silicon substrate for different geometries and material conditions. In particular, the effect of elastic mismatch between island and substrate is studied, yielding a profound understanding of the importance of the two modes describing the singular stress field.
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Chapter 1

Introduction

In microelectronic devices, strains are deliberately introduced into silicon to increase the mobility of electrons or holes; see Ref. [1] for a review. The strains, however, may cause mechanical failure. In particular, the devices usually contain sharp features like edges and corners, which may intensify strains and emit dislocations into silicon, ultimately failing the devices [2, 3].

Recently, a method was described to predict conditions under which such sharp features do not emit dislocations [4]. The method is further developed in the present report to account for split singularities [5, 6].

Figure 1.1: A blanket thin film, of thickness $h$ and residual stress, is grown on a (001) surface of a single-crystal silicon substrate. The film is then patterned into a stripe of width $L$, with the side surfaces parallel to the (110) plane of silicon.

Figure 1.1 illustrates the structure to be studied. A blanket film, of thickness $h$ and residual stress $\sigma$, is grown on the (001) surface of a single-crystal silicon substrate. The film is then patterned into a stripe of width $L$, with the side surfaces parallel to the (110) plane of silicon. When the film is patterned into a stripe, a field of stress builds up in the substrate, and
concentrates at the root of each edge. It is this concentrated stress that injects dislocations into silicon.

The structure in Figure 1.1 is similar to those studied in Refs. 4, 7-12, but this report will examine a specific aspect: split singularities. It is well known that, at the tip of a crack in a homogeneous elastic material, under plane strain conditions, the singular stress field is a linear superposition of two modes, the tensile mode and the shearing mode. More generally, at the tip of bonded wedges of dissimilar materials, the singular stress field may still consist of two modes, but usually of unequal exponents, either a pair of complex conjugates, or two unequal real numbers 6, 13-16. The case of complex-conjugate exponents has been extensively discussed within the context of a crack lying on a bimaterial interface 17. The present report will focus on the case that the two modes have unequal real exponents. That is, a stronger and a weaker singularity coexist. It has been shown that both singularities can be important in causing failure 5, 6, 16.

Chapter 2 describes the linear superposition of two modes of singular stress fields. Chapter 3 investigates which slip systems will be activated using crystallographic analysis. Chapter 4 calculates the critical residual stress in the thin-film stripe for injecting dislocations into the silicon substrate. Based on this sequence of analysis it is possible to predict critical dislocation planes and order of magnitude of the stress.
Chapter 2

Singular stress fields

Singular stress fields are present around infinitely sharp corners or features. In practice, a product feature can at most be atomistically sharp, which is less sharp than a theoretically sharp feature. However, singular stress calculations can play an important role in analyzing stress fields.

2.1 Dundurs parameters

The inset of Figure 2.1 illustrates an edge of a thin film bonded on a substrate, along with a system of polar coordinates \((r, \theta, z)\). In this view focused on the root of the edge, the film takes the quarter space, \(0^\circ \leq \theta \leq 90^\circ\), and the substrate takes the half space, \(-180^\circ \leq \theta \leq 0^\circ\). The two materials are bonded along the interface, \(\theta = 0^\circ\). Both materials are taken to be elastic and isotropic.

For problems of this type Dundurs [18] showed that the stress field depends on elastic constants through two dimensionless parameters:

\[
\alpha = \frac{\mu_f(1-\nu_s) - \mu_s(1-\nu_f)}{\mu_f(1-\nu_s) + \mu_s(1-\nu_f)} \tag{2.1}
\]

\[
\beta = \frac{1}{2} \frac{\mu_f(1-2\nu_s) - \mu_s(1-2\nu_f)}{\mu_f(1-2\nu_s) + \mu_s(1-2\nu_f)} \tag{2.2}
\]

where \(\mu\) is the shear modulus, and \(\nu\) Poisson’s ratio. The subscripts \(f\) and \(s\) refer to the film and the silicon substrate, respectively. By requiring \(0 \leq \nu \leq 0.5\) and \(\mu > 0\), the Dundurs parameters are confined within a parallelogram in the \((\alpha, \beta)\) plane, with vertices at \((1,0), (1,0.5), (-1,0)\) and \((-1,-0.5)\). In other words, Dundurs parameters represent the elastic mismatch.

For a singular field around the root of the edge, each component of the stress tensor, say \(\sigma_{\theta\theta}\), takes the form of \(\sigma_{\theta\theta} \sim r^\lambda\). This singular stress field is determined by an eigenvalue problem, resulting in a transcendental equation that determines the exponent \(\lambda\) [19–21]. The exponent is restricted to \(0 < Re(\lambda) < 1\), a restriction commonly adopted, with justifications criticized in Refs. [22,23]. For the specific geometry illustrated in the inset, Figure 2.1 plots...
Figure 2.1: The inset shows the root of an edge of a thin film bonded on a substrate. Contours of the singular exponents are plotted on the plane of the Dundurs parameters ($\alpha, \beta$). The parallelogram is divided into two regions by a bold curve. In the lower-left region, the exponents are two unequal real numbers, with the larger one labeled horizontally and the smaller one labeled vertically. In the upper-right region, the exponents are a pair of complex conjugates, with the real part depicted by solid lines and labeled horizontally, and the imaginary part depicted by dashed line and labeled vertically.

The contours of the exponents on the ($\alpha, \beta$) plane. The parallelogram is divided into two regions by a dark curve. In the lower-left region, the exponents are two unequal real numbers, one stronger ($\lambda_1$) and the other weaker ($\lambda_2$). The values for ($\lambda_1$) are labeled horizontally, and those for ($\lambda_2$) are labeled vertically. In the whole region, ($\lambda_2$) < ($\lambda_1$) ≤ 0.5. In the upper-right region, the exponents are a pair of complex conjugates, $\lambda_{1,2} = \xi \pm i\varepsilon$. The real part is depicted by solid lines and labeled horizontally, while the imaginary part is depicted by dashed lines and labeled vertically. At each point on the boundary (i.e., the dark curve), the two exponents degenerate to one number: when the point is approached from a region of real exponents, the two real exponents become identical; when the point is approached from a region of complex-conjugate exponents, the imaginary part vanishes. When $\alpha = 1$, i.e., the film is rigid, the singularity exponents are the same as those for an interfacial crack, $\lambda_{1,2} = 0.5 \pm i\varepsilon$, with $\varepsilon = 1/(2\pi)|ln[(1 - \beta)/(1 + \beta)]|$. [24]

As noted in Ref. [5], when the two materials have similar elastic constants, i.e., when $\alpha = \beta = 0$, the two modes of singular fields can be interpreted readily. In this case, the line bisecting the angle of the wedge is a line of symmetry. The stronger mode corresponds to a stress field symmetric about this line (i.e., the tensile mode). The weaker mode corresponds to a stress field anti-symmetric about this line (i.e., the shearing mode). When the two materials have dissimilar elastic constants, however, the symmetry is broken, and the two modes may not be interpreted in such a simple way.
In this report, $\alpha$ will be used to represent the elastic mismatch, and the effect of $\beta$ will be neglected by setting $\beta = 0$. When $\beta = 0$, the exponents are two unequal real numbers, regardless the values of $\alpha$. When setting $\beta = 0$ an assumption is made that is incorrect, because Poisson’s ratios are taken to be equal for the film and the substrate. Moreover material behavior is assumed to be incompressible, which is not correct for most materials used as films and substrates. This assumption is merely made in order to simplify the problem.

### 2.2 Linear superposition of two modes of singular stress fields

Several fundamental ideas in fracture mechanics are paraphrased [25]. Once the two unequal exponents are retained, the stress field around the root of the edge is a linear superposition of the two modes:

$$\sigma_{ij}(r, \theta) = \frac{k_1}{2\pi r^{\lambda_1}} \Sigma^{1}_{ij}(\theta) + \frac{k_2}{2\pi r^{\lambda_2}} \Sigma^{2}_{ij}(\theta)$$  \hspace{1cm} (2.3)

The angular functions $\Sigma^{1}_{ij}$ and $\Sigma^{2}_{ij}$ are normalized such that $\Sigma^{1}_{r\theta}(0) = \Sigma^{2}_{r\theta}(0) = 0$, and their full expressions are listed in Appendix A. The stress intensity factors, $k_1$ and $k_2$, are determined by the external boundary conditions, as described in Chapter 4.

The singular stress field (2.3) is obtained by assuming that the materials are elastic, and the edge is perfectly sharp. Such assumptions are invalid in a process zone around the root of the edge. Let $\Lambda$ be the size of the process zone, within which the singular stress field (2.3) is invalid. Also, the singular stress field (2.3) is invalid at size scale $h$, where the external boundary conditions will change the stress distribution. However, provided the process zone is significantly smaller than the macroscopic length, $\Lambda << h$, the singular stress field (2.3) prevails within an annulus, known as the $k$-annulus, of some radii bounded between $\Lambda$ and $h$.

The stress intensity parameters, $k_1$ and $k_2$, have different dimensions, $(stress)(length)^{\lambda_1}$ and $(stress)(length)^{\lambda_2}$, respectively. A convention is introduced by writing

$$k_1 = S\Lambda^{\lambda_1} \cos \psi, \quad k_2 = S\Lambda^{\lambda_2} \sin \psi$$  \hspace{1cm} (2.4)

This convention is illustrated in Figure 2.2. Here $S$ and $\psi$ characterize the stress field at length scale $\Lambda$, with $S$ characterizing the amplitude of the stress field, and $\psi$ characterizing the relative contribution of the two modes. Since both $k_1$ and $k_2$ can be either positive or negative, the mode angle can be in the entire range of $0^\circ \leq \psi \leq 360^\circ$.

The microscopic process of dislocation emission occurs within the process zone, but is driven by the stress field (2.3) in the $k$-annulus. Dislocations emit from the root when the amplitude $S$ reaches a critical value $S_c$, namely,

$$S(\psi) = S_c(\psi)$$  \hspace{1cm} (2.5)

The amplitude $S$ and the mode angle $\psi$ are determined by the external boundary conditions, by solving a boundary value problem of linear elasticity. The critical condition $S_c(\psi)$ is
determined either by experimental measurement or by computation from a microscopic model of the nucleation process.
Chapter 3

Selection of the critical slip system

Before numerical analysis can be performed, a profound understanding of the crystallographic orientation is a necessity. Twelve different slip systems exist within the silicon monocrystalline FCC-structure. In this chapter, slip systems are analyzed and the critical systems are determined.

3.1 Critical polar angle

Table 3.1 lists the twelve slip systems in silicon\[1\]. Given a mode angle, $\psi$, as the amplitude $S$ increases, some slip systems will activate earlier than others. We select the critical slip systems by the following procedure. For each slip system, we use the stress field Eq. (2.3) to calculate the resolved shear stress at distance $r = \Lambda$. The slip system with the maximum resultant shear stress is taken to be the critical slip system.

Table 3.1: The twelve slip systems and the corresponding critical polar angles are listed.

<table>
<thead>
<tr>
<th>Slip plane, $n$</th>
<th>Slip direction, $h$</th>
<th>Critical polar angle, $\theta^*$</th>
</tr>
</thead>
<tbody>
<tr>
<td>(111)</td>
<td>[110]</td>
<td>$-125, 26^\circ$</td>
</tr>
<tr>
<td></td>
<td>[101]</td>
<td>$-125, 26^\circ$</td>
</tr>
<tr>
<td></td>
<td>[011]</td>
<td>$-125, 26^\circ$</td>
</tr>
<tr>
<td>(1\bar{1}1)</td>
<td>[110]</td>
<td>$-54, 74^\circ$</td>
</tr>
<tr>
<td></td>
<td>[101]</td>
<td>$-54, 74^\circ$</td>
</tr>
<tr>
<td></td>
<td>[011]</td>
<td>$-54, 74^\circ$</td>
</tr>
<tr>
<td>(\bar{1}11)</td>
<td>[110]</td>
<td>$-54, 74^\circ$</td>
</tr>
<tr>
<td></td>
<td>[101]</td>
<td>$-54, 74^\circ$</td>
</tr>
<tr>
<td></td>
<td>[011]</td>
<td>$-125, 26^\circ$</td>
</tr>
</tbody>
</table>

\[1\] For slip systems $\frac{1}{2}(1\bar{1}1)[110]$ and $\frac{1}{2}(111)[110]$, the critical polar angle, i.e. the polar angle for which the resolved shear stress has a maximum, depends on the mode angle. This dependence is depicted in Figure 3.1.
For a given slip system, let $n_i$ be the unit vector normal to the slip plane, and $b_j$ be the Burgers vector. Under a general state of stress $\sigma_{ij}$, the resolved shear stress on the slip system is

$$\tau_{nb} = \frac{\sigma_{ij} n_i b_j}{b}$$

(3.1)

A combination of Eq. (2.3), Eq. (2.4) and Eq. (3.1) gives the resolved shear stress at the distance $r = \Lambda$ by

$$\frac{\tau_{nb}}{S} = |\cos(\psi) \frac{\Sigma_{ij}^1(\theta) n_i b_j}{(s\pi)^\lambda_1 b} + \sin(\psi) \frac{\Sigma_{ij}^2(\theta) n_i b_j}{(s\pi)^\lambda_2 b}|$$

(3.2)

Because this procedure only invokes the magnitude, not the direction, of the resolved shear stress, a simultaneous change in the sign of the two stress intensity factors $k_1$ and $k_2$ will not change the condition of dislocation emission. Consequently, we can restrict the range of the mode angle to $-90^\circ \leq \psi \leq 90^\circ$. Indeed, the right-hand side of Eq. (3.2) is a function of $\psi$ with a period of $360^\circ$.

An inspection of Figure 3.1 shows that the slip systems $\frac{1}{2}(111)[110]$ and $\frac{1}{2}(\overline{1}11)[110]$ are of zero resolved shear stress. The slip systems $\frac{1}{2}(111)[10\overline{1}]$ and $\frac{1}{2}(1\overline{1}1)[01\overline{1}]$ are of identical resolved shear stress and with fixed polar angle $-125.26^\circ$. Other similar pairs of slip systems are listed in Table 3.1. By contrast, the resolved shear stress for slip systems $\frac{1}{2}(1\overline{1}1)[110]$ and $\frac{1}{2}(\overline{1}11)[110]$ is a function of polar angle $\theta$. As an example, in Figure 3.1a, the resolved shear stress is plotted as a function of $\theta$. The polar angle $\theta^*$ corresponding to the maximum resolved shear stress is selected as the critical angle where the potential dislocation is nucleated. In (b), all the critical polar angles $\theta^*$ in the range $-90^\circ \leq \psi \leq 90^\circ$ are plotted for $\alpha = 0.5$.  

Figure 3.1: The normalized resolved shear stress for slip systems $\frac{1}{2}(1\overline{1}1)[110]$ and $\frac{1}{2}(\overline{1}11)[110]$ is a function of the polar angle $\theta$. As an example, in (a), the normalized shear stress is plotted as a function of $\theta$. The polar angle $\theta^*$ corresponding to the maximum resolved shear stress is selected and marked by ”x” as the critical angle where the potential dislocation is nucleated. In (b), all the critical polar angles $\theta^*$ in the range $-90^\circ \leq \psi \leq 90^\circ$ are plotted for $\alpha = 0.5$.  

An inspection of Figure 1.1 shows that the slip systems $\frac{1}{2}(111)[110]$ and $\frac{1}{2}(\overline{1}11)[110]$ are of zero resolved shear stress. The slip systems $\frac{1}{2}(111)[10\overline{1}]$ and $\frac{1}{2}(1\overline{1}1)[01\overline{1}]$ are of identical resolved shear stress and with fixed polar angle $-125.26^\circ$. Other similar pairs of slip systems are listed in Table 3.1. By contrast, the resolved shear stress for slip systems $\frac{1}{2}(1\overline{1}1)[110]$ and $\frac{1}{2}(\overline{1}11)[110]$ is a function of polar angle $\theta$. As an example, in Figure 3.1a, the resolved shear stress is plotted as a function of $\theta$ for $\psi = 0$ and $\alpha = 0.5$. The polar angle $\theta^*$ corresponding to the maximum resolved shear stress is selected as the critical angle where the
potential dislocation is nucleated. In Figure 3.1b, the critical polar angle $\theta^*$ in the loading range $-90^\circ \leq \psi \leq 90^\circ$ is plotted for $\alpha = 0.5$. This procedure can be repeated for all values of $\alpha$.

Fig. 3.2 shows how Fig. 3.1b relates to three dimensions in the case of $\alpha = 0.5$, Fig. 3.1b shows where in the base plane of Fig. 3.2 the maximum values for the normalized resolved shear stress are occurring. Ultimately, it is important to know the maximum resolved shear stress of the slip systems $\frac{1}{2}(1\bar{1}1)[110]$ and $\frac{1}{2}(T11)[110]$ in order to determine which slip systems are critical. Here, Fig. 3.1b provides the necessary input for the calculation of the critical slip system and implicitly completes Table 3.1.

Figure 3.2: Normalized resolved shear stress as a function of the polar angle, $\theta$ and the mode angle, $\psi$ for $\alpha = 0.5$ for slip systems $\frac{1}{2}(1\bar{1}1)[110]$ and $\frac{1}{2}(T11)[110]$.

3.2 Maximum resolved shear stress

For $\alpha = 0.5$, Fig. 3.3a plots the resolved shear stresses as a function of the mode angle $\psi$ for all twelve slip systems. The slip system with largest resolved shear stress is the potential slip system on which dislocations are firstly injected. The slip systems so selected are marked as the critical slip system for the whole range value of $-90^\circ \leq \psi \leq 90^\circ$. Obviously, different slip systems can be activated for different values of mode angle $\psi$. Similarly, the critical slip systems for any material combination under any mode angle can be selected, such as shown in Fig. 3.3b for $\alpha = 0$ and in Fig. 3.3c for $\alpha = -0.5$. 

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Figure 3.3: Normalized resolved shear stresses are plotted as a function of mode angle for all twelve slip systems. The slip system with the largest resolved shear stress is the potential slip system on which the dislocation is nucleated first, so those slip systems are selected and marked for the whole range of the mode angle, $-90^\circ \leq \psi \leq 90^\circ$. (a) $\alpha = 0.5$ (b) $\alpha = 0$ (c) $\alpha = -0.5$. 
Chapter 4

The critical condition for dislocation emission

The stress field around the root of the edge is described by Eq. [2.3]. Linearity and dimensional consideration dictate that the stress intensity factors $k_1$ and $k_2$ should take the form

$$k_1 = \sigma h^{\lambda_1} f_1(L/h, \alpha), \quad k_2 = \sigma h^{\lambda_2} f_2(L/h, \alpha)$$ (4.1)

where the dimensionless functions $f_1(L/h, \alpha)$ and $f_2(L/h, \alpha)$ are determined using curve fitting. The full stress field is calculated in the structure by using the finite element package ABAQUS.
4.1 Finite element analysis

The finite element method is applied in order to calculate the stress field of the entire structure. The schematic representation of the structure is depicted in Fig. 4.1. It is necessary to determine the entire stress field in the problem at hand, because we need the values for the interfacial shear stress for the analysis.

![Figure 4.1: Overview of the mesh used in the fully elastic FE analysis. The mesh is depicted at different scales for $L/h = 20$ with a) the total mesh b) the total island c) island scale ($h = 1$) d) smallest detail ($10^{-4}$)](image)

Fig. 4.1 depicts the mesh used in the ABAQUS finite element analysis at different scales. The geometry is divided into several geometrical subsets. Once again, it is the interfacial shear stress near the root that is of interest. The curve fit is based upon the stress field within the process zone [6].
4.2 Curve fitting

The next step is to fit the interfacial shear stress close to the root \([6]\), say \(10^{-3} < r/h < 10^{-2}\), to the equation

\[
\sigma_{r\theta}(\theta = 0) = \frac{k_1}{(2\pi r)^{\lambda_1}} + \frac{k_2}{(2\pi r)^{\lambda_2}}
\]  
(4.2)

with \(k_1\) and \(k_2\) as fitting parameters. The two functions so calculated are plotted in Fig. 4.2. Although the stress field intensifies at the root, the side surface of the stripe is traction-free. When the stripe is very narrow, \(L/h \to 0\), the stress in the stripe is almost fully relaxed. When the stripe is very wide, \(L/h \to \infty\), the stress field near one edge of the stripe no longer feels the presence of the other edge, so \(f_1\) and \(f_2\) attain plateaus.

![Figure 4.2: The normalized stress intensity factors, \(f_1\) and \(f_2\), are plotted as a function of the aspect ratio, \(L/h\), of the stripe on the silicon substrate.](image)

A combination of Eq. 2.4 and Eq. 4.1 gives the mode angle \(\psi\) as

\[
tan(\psi) = \frac{f_2}{f_1} \left(\frac{\Lambda}{h}\right)^{\lambda_1 - \lambda_2}
\]  
(4.3)

Take the typical value of film thickness \(h = 100 \text{ nm}\), and take the process zone size \(\Lambda\) to be the Burgers vector in silicon \(b = 0, 383 \text{ nm}\). Fig. 4.3 plots the mode angle \(\psi\) as a function of the Dundurs parameter \(\alpha\) for aspect ratio of the stripe, \(L/h = 2\) and \(L/h = 20\). We observe that for the values of \(\alpha < 0\), i.e. when the film is more compliant than the substrate, both the elastic mismatch and the aspect ratio have negligible effects on the mode angle \(\psi\), and the weaker singular term in Eq. 2.3 is negligible, so that the singular stress field in Eq. 2.3 can be simplified to the single mode. However, for positive values of \(\alpha\), i.e., when the film is stiffer than the substrate, the mode angle \(\psi\) increases rapidly, and both singular terms in Eq. 2.3 should be taken into account.

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As a comment on the case studied in Ref. [4], the film stripe is SiN with shear modulus 54.3 GPa and Poisson’s ratio $\nu = 0.27$. The silicon substrate is of shear modulus 68.1 GPa and Poisson’s ratio $\nu = 0.22$. The elastic mismatch is small, $\alpha \approx 0$. The singularity exponents are $\lambda_1 = 0.4514$ and $\lambda_2 = 0.0752$. Still taking $h = 100 \, nm$ and $b = 0.383 \, nm$, we obtain that $\psi = 0, 2^\circ$ for $L/h = 20$, and $\psi = 1, 27^\circ$ for $L/h = 2$. Evidently in this case the weaker singularity has a negligible contribution. From Fig. 3.2(b), we identify the critical slip systems as $\frac{1}{2}(111)[01\bar{1}]$ and $\frac{1}{2}(111)[10\bar{1}]$, which is predicted in Ref. [4].

### 4.3 Critical stress

The critical residual stress in the thin-film stripe to inject dislocations into silicon are calculated. It is assumed that the critical condition is reached when the maximum resolved shear stress reaches the theoretical shear strength at distance $r = b$. The theoretical shear strength is estimated by $\tau_{th} = 0.2\mu$, where $\mu$ is the shear modulus of silicon. Setting $\tau_{th}(b) = \tau_{th}$, a combination of Eqs. 2.3, 3.1 and 4.1 gives a scaling relation between the critical residual stress and the feature sizes:

$$\frac{\sigma_c}{\mu} = 0, 2\left\{ \left[ \left( \frac{h}{b} \right)^{\lambda_1} \frac{\Sigma_{ij}^1}{(2\pi)^{\lambda_1}} f_1 + \left( \frac{h}{b} \right)^{\lambda_2} \frac{\Sigma_{ij}^2}{(2\pi)^{\lambda_2}} f_2 \right] \frac{n_i b_j}{b} \right\}^{-1} \quad (4.4)$$

Figs. 3.3 and 4.3 show that the critical slip systems are $\frac{1}{2}(111)[01\bar{1}]$ and $\frac{1}{2}(111)[10\bar{1}]$.

In Fig. 4.3 the normalized critical stresses are plotted as a function of the aspect ratio, $L/h$, for Dundurs $\alpha = 0.5$, $\alpha = 0$, $\alpha = -0.5$. A plateau is reached for large values of the aspect ratio $L/h$. When the aspect ratio is decreased, the critical stress will drastically
improve, implying the fact that a narrow stripe might not inject dislocations into the silicon substrate, while a wide stripe could inject dislocations. Also evident is that the critical stress increases as the film becomes stiffer. This is because the same level of residual stress in a stiff film will induce a low level of stress if the substrate is relatively compliant.

Figure 4.4: Normalized critical stresses are plotted as a function of the aspect ratio $L/h$ for Dundurs parameter $\alpha = 0.5$, $\alpha = 0$, $\alpha = -0.5$. 
Chapter 5

Conclusion

The singular stress field at the root of an edge is a linear superposition of two modes, with different exponents. A mode angle $\psi$ is introduced to measure the relative contribution of the two modes to the failure conditions. Fig 2.1 shows that the two exponents are different when the film is compliant relative to silicon, and are similar when the film is stiff relative to silicon. Consequently, as shown in Fig. 4.3, the weaker singular field is negligible when the film is compliant, but is significant when the film is stiff.

For the full range of the mode angle, a procedure is described to select the critical slip systems. On the basis of the criterion that dislocations nucleate when the resolved shear stress at distance $b$ from the root of the thin-film edge reaches the theoretical strength, we calculate the critical residual stress in the stripe, and show that the critical stress is low when the stripe is wide or compliant.
Appendix A

Stress components

The singular stress field Eq. (2.3) is solved by the methods outlined in Ref. [10, 5]. The eigenfunctions $\Sigma_{ij}(\theta)$ associated with the eigenvalue $\lambda$ are expressed in polar coordinates $(r, \theta, z)$ as

$$\Sigma_{rr}(\theta) = - (\lambda - 1)(\lambda - 2)[Asin(\lambda - 2)\theta + Bcos(\lambda - 2)\theta] + (\lambda + 2)[Csin\lambda\theta + Dcos\lambda\theta]$$

$$\Sigma_{\theta\theta}(\theta) = (\lambda - 1)(\lambda - 2)[Asin(\lambda - 2)\theta + Bcos(\lambda - 2)\theta + Csin\lambda\theta + Dcos\lambda\theta]$$

$$\Sigma_{r\theta}(\theta) = (\lambda - 1)(\lambda - 2)[Asin(\lambda - 2)\theta - Bcos(\lambda - 2)\theta] + \lambda[Ccos\lambda\theta - Dsin\lambda\theta]$$

$$\Sigma_{zz}(\theta) = -4\nu(\lambda - 1)[Csin\lambda\theta + Dcos\lambda\theta]$$

$$\Sigma_{r\theta}(\theta) = \Sigma_{\theta z}(\theta) = 0$$

The eigenvalue $\lambda$ and its associated coefficients $A$, $B$, $C$ and $D$ in the film and the substrate are solved by the boundary conditions. In this paper, the singular stress field in the silicon substrate around the root of the edge causes dislocation to be emitted, so that the eigenvalues and the associated coefficients only in the substrate are listed in Table A.1 (for $\alpha = 0.5$, $\alpha = 0$, $\alpha = -0.5$ with $\beta = 0$).

Table A.1: Singularity exponents and the associated coefficients in Eqs A.1 in silicon substrate for $\alpha = 0.5$, $\alpha = 0$, $\alpha = -0.5$ with $\beta = 0$.

<table>
<thead>
<tr>
<th>$\alpha$</th>
<th>0.5</th>
<th>0</th>
<th>-0.5</th>
<th>0</th>
<th>0.5</th>
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</thead>
<tbody>
<tr>
<td>$\lambda$</td>
<td>0.4314</td>
<td>0.4555</td>
<td>0.4783</td>
<td>0.2542</td>
<td></td>
</tr>
<tr>
<td>$A$</td>
<td>0.9803</td>
<td>0.9885</td>
<td>0.9951</td>
<td>0.4213</td>
<td></td>
</tr>
<tr>
<td>$B$</td>
<td>-0.2687</td>
<td>-0.3775</td>
<td>-0.1427</td>
<td>-0.6517</td>
<td>-0.9088</td>
</tr>
<tr>
<td>$C$</td>
<td>-0.5123</td>
<td>-0.6804</td>
<td>-0.8414</td>
<td>-0.2542</td>
<td></td>
</tr>
<tr>
<td>$D$</td>
<td>1.8693</td>
<td>1.8201</td>
<td>1.7750</td>
<td>-1.1040</td>
<td></td>
</tr>
</tbody>
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Appendix B

Crystal coordinate transformation

In calculating the resolved shear stress Eq. (3.1), the stress components in the crystal coordinates ($x_1, x_2, x_3$), $\sigma_{ij}$, are converted from those in the polar coordinates ($r, \theta, z$). The relation of ($x_1, x_2, x_3$) and ($r, \theta, z$) is depicted in Fig. 1.1, and the matrix of conversion is

$$[Q] = \begin{pmatrix} \frac{-\cos\theta}{\sqrt{2}} & \frac{-\cos\theta}{\sqrt{2}} & \text{sin}\theta \\ \frac{-\cos\theta}{\sqrt{2}} & \frac{-\cos\theta}{\sqrt{2}} & \text{cos}\theta \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \end{pmatrix}$$ (B.1)

From $[\sigma]_{\text{crystal}} = [Q]^T[\sigma]_{\text{polar}}[Q]$, the stress components in crystal coordinates are

$$\sigma_{11} = \sigma_{22} = \frac{(\sigma_{rr}\text{cos}^2\theta + \sigma_{\theta\theta}\text{sin}^2\theta + \sigma_{zz} - \sigma_{r\theta}\text{sin}2\theta)}{2} \quad \text{(B.2)}$$

$$\sigma_{12} = \sigma_{21} = \frac{(\sigma_{rr}\text{cos}^2\theta + \sigma_{\theta\theta}\text{sin}^2\theta - \sigma_{zz} - \sigma_{r\theta}\text{sin}2\theta)}{2} \quad \text{(B.3)}$$

$$\sigma_{13} = \sigma_{31} = \sigma_{23} = \frac{[(\sigma_{\theta\theta} - \sigma_{rr})\text{sin}2\theta - 2\sigma_{r\theta}\text{cos}2\theta]}{2\sqrt{2}} \quad \text{(B.4)}$$

$$\sigma_{33} = \sigma_{rr}\text{sin}^2\theta + \sigma_{\theta\theta}\text{cos}^2\theta + \sigma_{r\theta}\text{sin}2\theta \quad \text{(B.5)}$$
References


