ANALYSIS OF SILICON STRESS/STRAIN RELATIONSHIPS

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O. Dillon

Dislocation Density Contour Plot

\[ T = 1412 - 110.74 \times X + 3.5 \times X^2 \]

UNIT OF X AND Y = CM. Z = 1 PER CM^2

Dislocation density contour plot for the parabolic thermal profile of Eq. (4-6), 8x7 cm ribbon and an initial dislocation density = 0.5 cm^-2.
Dislocation Density Along $Y = 0$ (Centerline)

$T = 1412 - 110.74X + 3.5X^2$

LINE 1 FOR WIDTH = 8 CM  LINE 2 FOR WIDTH = 7 CM
LINE 3 FOR WIDTH = 6 CM  LINE 4 FOR WIDTH = 4 CM

Dislocation density along the centerline of the ribbon for the parabolic thermal profile of Eq. (4-8), initial dislocation density = 0.5 cm$^{-2}$, and width = 8, 7, 6, 4 cm.
ADVANCED SILICON SHEET

Final Dislocation Density Along the Ribbon
Width for Westinghlcuse Profile

LENGTH = 12 CM, WIDTH = 3.5 CM
STAR FJR NO = 13 /CMxmm2
DIAMOND FOR NO = 5 /CMxmm2
SQUARE FOR NO = 1 /CMxmm2

No = 13/cm²
No = 5/cm²
No = 1/cm²
ADVANCED SILICON SHEET

Dislocation Density Contour Plot

WESTINGHOUSE PROFILE, NO=0.25/CM^2, R/T=0
UNIT OF X AND Y=CM, Z=1 PER CM^2

LEGEND: Z

\[
\begin{align*}
&10 \quad 201 \\
&39 \quad 583 \\
&774 \quad 965 \\
&1156 \quad 1347 \\
&1538 \quad 1729 \\
&1920 \quad 2111 \\
&2302 \quad 2493 \\
&2684
\end{align*}
\]
Dislocation Density Contour Plot

WESTINGHOUSE PROFILE, NO=0.375/CMX2
UNIT OF X AND Y=CM, Z=1/CMX2, A/T=1.6667 M

LEGEND: Z

<table>
<thead>
<tr>
<th>Z</th>
<th>130</th>
<th>750</th>
<th>1370</th>
<th>1990</th>
<th>2610</th>
<th>3230</th>
<th>3850</th>
<th>4470</th>
</tr>
</thead>
<tbody>
<tr>
<td>Note Low Densities</td>
<td>440</td>
<td>1060</td>
<td>1660</td>
<td>2300</td>
<td>2920</td>
<td>3540</td>
<td>4160</td>
<td></td>
</tr>
</tbody>
</table>

with Deformities

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Advanced Silicon Sheet

Effective Plastic Strain Rate

Westinghouse Profile, NO=0.25/cm×2
Width = 6 cm, Length = 8 cm, A/T=0.
Unit of X and Y=cm, Z=10××-5 per sec

Plastic Strain Rate

No dendrites

Outside
ADVANCED SILICON SHEET

Effective Plastic Strain Rate

WESTINGHOUSE PROFILE, NO = 0.375/CM, T=2
WIDTH = 6 CM, LENGTH = 8 CM, R/T = 1.6667 MM
UNIT OF X AND Y = CM, Z = 10^-5 PER SEC

PLASTIC STRAIN RATE

![Graph of Plastic Strain Rate]

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ADVANCED SILICON SHEET

Residual Stress XX Along Ribbon
Width for Westinghouse Profile

LENGTH = 12 CM, WIDTH = 3.5 CM
STAR FOR NO = 13 /CM×2
DIAMOND FOR NO = 5 /CM×2
SQUARE FOR NO = 1 /CM×2

No = 13/cm²
No = 5/cm²
No = 1/cm²
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Deflection Shape

MILE-WIDTH \( C_1 = 1 \), LENGTH = 8.0
DIAMETER OF DENDRITES IS 0.0 INCHES
CRITICAL THICKNESS = 0.00526 INCHES

\[ T(x) = \text{parabola} \]
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Deflection Shape

HALF-WIDTH (C) = 1., LENGTH = 6.0
DIAMETER OF DENDRITES IS 0.2 INCHES
CRITICAL THICKNESS = 0.057120 INCHES

\[ T(x) = \text{parabolic} \]
Topics

1 Dislocation Motion

A) Problem Formulation
B) Calculation of Forces
C) Tracking the motion of a single Dislocation

2 Dislocation Multiplication & Density

A) Three methods of calculations - based on resolved shear stresses on each slip system

B) Dislocation density by averaging the | shear stresses | in 0.5 cm. widths of ribbon. (starting at x = 0.2 cm.)
### Possible Dislocations in the Silicon Crystal

<table>
<thead>
<tr>
<th>Burgers vector</th>
<th>Tangent vector</th>
<th>Slip plane</th>
<th>Type of dislocation</th>
</tr>
</thead>
<tbody>
<tr>
<td>&lt;-1 0 -1&gt;</td>
<td>&lt;-1 0 -1&gt;</td>
<td>(-1 -1 1), left, screw</td>
<td></td>
</tr>
<tr>
<td>=</td>
<td>&lt;0 1 1&gt;</td>
<td>left, 60' (-120') ✓</td>
<td></td>
</tr>
<tr>
<td>=</td>
<td>&lt;1 -1 0&gt;</td>
<td>left, 60' (+120') ✓</td>
<td></td>
</tr>
<tr>
<td>=</td>
<td>&lt;1 -2 -1&gt;</td>
<td>left, edge</td>
<td></td>
</tr>
<tr>
<td>&lt;0 1 1&gt;</td>
<td>&lt;0 1 1&gt;</td>
<td>left, screw</td>
<td></td>
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<td>=</td>
<td>&lt;-1 0 -1&gt;</td>
<td>left, 60' (-120') ✓</td>
<td></td>
</tr>
<tr>
<td>=</td>
<td>&lt;-2 1 -1&gt;</td>
<td>left, edge</td>
<td></td>
</tr>
<tr>
<td>&lt;-1 1 0&gt;</td>
<td>&lt;-1 1 0&gt;</td>
<td>left, screw</td>
<td></td>
</tr>
<tr>
<td>=</td>
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<td>=</td>
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<td></td>
</tr>
<tr>
<td>=</td>
<td>&lt;-1 1 -2&gt;</td>
<td>left, edge</td>
<td></td>
</tr>
<tr>
<td>&lt;1 0 -1&gt;</td>
<td>&lt;1 0 -1&gt;</td>
<td>(-1 1 -1), right, screw</td>
<td></td>
</tr>
<tr>
<td>=</td>
<td>&lt;-1 -1 0&gt;</td>
<td>right, 60' (-120') ✓</td>
<td></td>
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<td>=</td>
<td>&lt;1 -2 -1&gt;</td>
<td>right, edge</td>
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</tr>
<tr>
<td>&lt;-1 1 0&gt;</td>
<td>&lt;-1 1 0&gt;</td>
<td>right, screw</td>
<td></td>
</tr>
<tr>
<td>=</td>
<td>&lt;1 0 1&gt;</td>
<td>right, 60' (+120')</td>
<td></td>
</tr>
<tr>
<td>=</td>
<td>&lt;-1 2 -1&gt;</td>
<td>right, edge</td>
<td></td>
</tr>
<tr>
<td>&lt;1 1 0&gt;</td>
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<td></td>
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<td></td>
</tr>
<tr>
<td>=</td>
<td>&lt;0 -1 -1&gt;</td>
<td>right, 60' (-120') ✓</td>
<td></td>
</tr>
<tr>
<td>=</td>
<td>&lt;-1 1 -2&gt;</td>
<td>right, edge</td>
<td></td>
</tr>
<tr>
<td>&lt;0 -1 1&gt;</td>
<td>&lt;-0 -1 1&gt;</td>
<td>(-1 1 -1), transv., screw</td>
<td></td>
</tr>
<tr>
<td>=</td>
<td>&lt;1 1 0&gt;</td>
<td>transv., 60' (+120') ✓</td>
<td></td>
</tr>
<tr>
<td>=</td>
<td>&lt;-1 0 -1&gt;</td>
<td>transv., 60' (-120') ✓</td>
<td></td>
</tr>
<tr>
<td>=</td>
<td>&lt;2 1 1&gt;</td>
<td>transv., edge</td>
<td></td>
</tr>
<tr>
<td>&lt;1 1 0&gt;</td>
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<tr>
<td>=</td>
<td>&lt;-1 -1 2&gt;</td>
<td>transv., edge</td>
<td></td>
</tr>
<tr>
<td>&lt;1 0 1&gt;</td>
<td>&lt;1 0 1&gt;</td>
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<td>=</td>
<td>&lt;-1 -2 1&gt;</td>
<td>transv., edge</td>
<td></td>
</tr>
</tbody>
</table>

1. Surface of the ribbon is (1 1 1) plane.
2. Growth direction to the melt is <-2 1 -1>.
3. For the motion of the dislocations, 60' dislocations that have -120 degree with the burgers vector will be chosen because these 60' dislocations may multiply themselves more than +120' type 60' dislocations as many investigators observed.
Assumptions

(1) The density of dislocation at the liquid solid interface is uniform.

(2) The pulling rate of the ribbon is 3 cm/min.

(3) Dislocations can move only in active slip systems that have their resolved shear stress higher than 95% of the most active slip system that has maximum Schmid Factor.

(4) Average velocity of the dislocations in the presence of other dislocations is almost same as the velocity of isolated dislocation.

Equivalent to low dislocation density.

(5) The velocity equation proposed by K. Sumino

\[ V = V_0 \tau \exp(-E/kT) \]

where \( E \) is 2.2 eV for 60' and 2.35 eV for screw,

\[ V_0 \text{ is } 0.035 \text{ for screw and } 0.01 \text{ m}^3/\text{MN.s} \text{ for 60'.} \]

is still valid at high temperature like around melting temperature.
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Resolved Shear Stress

Sign Change

$\Delta x = 0.125$

Legend:

-9247885
-7022960
-4987785
3102395
-1877940

Left
Motion of Dislocation

$B=b/2 (-1, 1 0), T=(1 0 1), M=(-1 -1 1)$

UNIT OF AXES ARE CM
Motion of the Dislocations Emerging to the Surface

<table>
<thead>
<tr>
<th>Burger's Vector</th>
<th>Tangent Vector</th>
<th>Plane</th>
<th>Motion</th>
</tr>
</thead>
<tbody>
<tr>
<td>( a/2(-1 0 -1) )</td>
<td>( (0 1 1) )</td>
<td>(-1 -1 1)</td>
<td>Left Strong</td>
</tr>
<tr>
<td>( a/2(-1 1 0) )</td>
<td>( (0 -1 -1) )</td>
<td>(-1 -1 1)</td>
<td>*</td>
</tr>
<tr>
<td>( a/2(-1 1 0) )</td>
<td>( (1 0 1) )</td>
<td>(-1 -1 1)</td>
<td>Split</td>
</tr>
<tr>
<td>( a/2(0 1 1) )</td>
<td>(-1 0 -1)</td>
<td>(-1 -1 1)</td>
<td>Right Weak</td>
</tr>
<tr>
<td>( a/2(1 0 -1) )</td>
<td>( (0 1 1) )</td>
<td>(-1 1 -1)</td>
<td>Right Strong</td>
</tr>
<tr>
<td>( a/2(1 0 -1) )</td>
<td>(-1 -1 0)</td>
<td>(-1 1 -1)</td>
<td>*</td>
</tr>
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<td>( a/2(1 1 0) )</td>
<td>( (0 -1 -1) )</td>
<td>(-1 1 -1)</td>
<td>*</td>
</tr>
<tr>
<td>( a/2(0 -1 -1) )</td>
<td>( (1 1 0) )</td>
<td>(-1 1 -1)</td>
<td>Right Weak</td>
</tr>
<tr>
<td>( a/2(0 -1 1) )</td>
<td>(-1 0 -1)</td>
<td>(1 -1 -1)</td>
<td>Right Strong</td>
</tr>
<tr>
<td>( a/2(0 -1 1) )</td>
<td>(-1 -1 0)</td>
<td>(1 -1 -1)</td>
<td>Left Strong</td>
</tr>
<tr>
<td>( a/2(1 0 1) )</td>
<td>(-1 -1 0)</td>
<td>(1 -1 -1)</td>
<td>Left Weak</td>
</tr>
<tr>
<td>( a/2(1 1 0) )</td>
<td>(-1 0 -1)</td>
<td>(1 -1 -1)</td>
<td>Left Weak</td>
</tr>
</tbody>
</table>

*; These are forced into the liquid
Calculation of the Density of Dislocations

From the K. Sumino's equation of dislocation multiplication

\[ \frac{dN_m}{dt} = K K_0 N_m^1 (T_a - G b \sqrt{N_m^2 / \beta})^{(m + \lambda)} \exp(-Q/kT) \]

where \( K, K_0, b, \beta, m, \lambda, k, Q \) are constants given by K. Sumino

- \( N_m^1 \) is dislocation density
- \( N_m^1 \propto \) source density
- \( N_m^2 \) is the density controlling the back stress

\( T_a \); applied stresses
\( T \); temperature
\( G \); shear modulus
\( t \); time

Three possible ways of application of the equation (A)

1. \( N_m^1 \) and \( N_m^2 \) are total density of dislocations

2. \( N_m^1 \) is the partial density of dislocations on each slip system and
   \( N_m^2 \) is the total density of dislocations.

3. Both \( N_m^1 \)'s are partial densities of dislocations on each slip system
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Method Calculating Dislocation Density

\[ N_{m1} \quad N_{m2} \]

(1) \( \downarrow \rightarrow \text{RSS}_i \quad \upharpoonright \quad \text{total density} = N_{m1} = N_{m2} \)

\[ dN_{m} = dN_{m1} = dN_{m2} \]

(2) \( \downarrow \rightarrow \text{RSS}_i \quad \upharpoonright \quad \text{total density} = \sum_\ell (N_{m1})_i = N_{m2} \)

\[ dN_{m2} = \sum_\ell (dN_{m})_i \]

(3) \( \downarrow \rightarrow \text{RSS}_i \quad \upharpoonright \quad \text{total density} = \sum_\ell (N_{m1})_i = \sum_\ell (N_{m2})_i \)

\[ (dN_{m1})_i = (dN_{m2})_i \]
Total Density of Dislocation Using YI, YTOT and DGGEAR

INITIAL TOTAL DENSITY IS 90/M=2 LAMBDA IS 1.0

Y

LEGEND: DENS
- 8.5915E+17
- 6.014E+18
- 1.1169E+19
- 1.6324E+19

T

0.00 0.15 0.30 0.45 0.60 0.75 0.90 1.05 1.20 1.35 1.50

0.0 0.2 0.4 0.6 0.8 1.0 1.2 1.4 1.6 1.8 2.0
Total Density of Dislocation Using YI, YI and DGEAR

Initial Total Density is 90/mm², LAMDA is 1.0

Legend: DENS 8 7.7220E+11 5.4054E+12 3.0888E+12 3.7220E+12 1.7448E+14 1.7448E+14
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Averaging the $|\tau a|$ in Calculating Density

---

center  edge

column 1 ; * , column 2 ; • column 3 ; □
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Nine Slip Systems

<table>
<thead>
<tr>
<th>burger's vector</th>
<th>slip plane</th>
<th>type of plane</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a/2 \begin{pmatrix} 1 &amp; 0 &amp; 1 \end{pmatrix}$</td>
<td>$(1 \ -1 \ -1)$</td>
<td>left</td>
</tr>
<tr>
<td>$a/2 \begin{pmatrix} 0 &amp; 1 &amp; 1 \end{pmatrix}$</td>
<td>$(1 \ -1 \ -1)$</td>
<td>left</td>
</tr>
<tr>
<td>$a/2 \begin{pmatrix} -1 &amp; 1 &amp; 0 \end{pmatrix}$</td>
<td>$(1 \ -1 \ -1)$</td>
<td>left</td>
</tr>
<tr>
<td>$a/2 \begin{pmatrix} 1 &amp; 0 &amp; -1 \end{pmatrix}$</td>
<td>$(1 \ 1 \ -1)$</td>
<td>right</td>
</tr>
<tr>
<td>$a/2 \begin{pmatrix} 1 &amp; 1 &amp; 0 \end{pmatrix}$</td>
<td>$(1 \ 1 \ -1)$</td>
<td>right</td>
</tr>
<tr>
<td>$a/2 \begin{pmatrix} 0 &amp; 1 &amp; 1 \end{pmatrix}$</td>
<td>$(1 \ -1 \ -1)$</td>
<td>right</td>
</tr>
<tr>
<td>$a/2 \begin{pmatrix} 0 &amp; -1 &amp; 1 \end{pmatrix}$</td>
<td>$(1 \ -1 \ -1)$</td>
<td>transverse</td>
</tr>
<tr>
<td>$a/2 \begin{pmatrix} 1 &amp; 0 &amp; 1 \end{pmatrix}$</td>
<td>$(1 \ -1 \ -1)$</td>
<td>transverse</td>
</tr>
<tr>
<td>$a/2 \begin{pmatrix} 1 &amp; 1 &amp; 0 \end{pmatrix}$</td>
<td>$(1 \ -1 \ -1)$</td>
<td>transverse</td>
</tr>
</tbody>
</table>
Density of Dislocations When NO is 1 at \( x = 0.2 \text{ cm} \)

\[ t = b \]

UNIT OF \( x \) IS CM, \( z \) IS DENSITY IN \( 1/\text{m}^2 \)
Density of Dislocations When NO is 1 at x = 0.2 cm

UNIT OF X IS CM, Z IS DENSITY IN 1/M**2
ADVANCED SILICON SHEET

Density of Dislocations When NO is 1 at \( x = 0.2 \text{ cm} \)

UNIT OF X IS CM, Z IS DENSITY IN \( 1/M^{**2} \)
Dislocation Multiplication by Stress Averaging Over 0.5 cm

<table>
<thead>
<tr>
<th>Dislocation Type</th>
<th>Multiplication Factor</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Center</td>
</tr>
<tr>
<td>[101] [111] L</td>
<td>750</td>
</tr>
<tr>
<td>[011] [111] L</td>
<td>2.5</td>
</tr>
<tr>
<td>[110] [111] L</td>
<td>23</td>
</tr>
<tr>
<td>[110] [111] R</td>
<td>750</td>
</tr>
<tr>
<td>[101] [111] R</td>
<td>12</td>
</tr>
<tr>
<td>[011] [111] R</td>
<td>1</td>
</tr>
<tr>
<td>[101] [111] T</td>
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</tr>
<tr>
<td>[110] [111] T</td>
<td>2</td>
</tr>
<tr>
<td>[011] [111] T</td>
<td>1.5</td>
</tr>
</tbody>
</table>

Calculations started at x=0.2 cm.

[Diagram of dislocation type and multiplication factor areas]
Dislocation Distribution in Web Dendrite Ribbon
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Cz Temperature Dependence

Cz Strain Rate Dependence
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Cz Temperature Dependence

![Graph showing temperature dependence of Cz growth.](image)

Web Ribbon: Strain Rate Dependence

![Graph showing strain rate dependence of web ribbon.](image)
Web Ribbon: Temperature Dependence

![Graph showing temperature dependence of R.S. stress. The graph plots R.S. stress (0.2% offset/δ/μ) in MPa against 1000/T (°C) with markers for strain rates of 1E-04 and 1E-05. The line equation is given as S = N * e^(-E_a/R_μ) where N = 2 x 10^4 m^-1 and E_a = 1.2 x 10^5 J mol^-1.]