ANALYSIS OF SILICON STRESS/STRAIN RELATIONSHIPS

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O. Dillon

Dislocation Density Contour Plot

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

UNIT OF X AND Y = CM, \( Z = 1 \) PER CM^2

Dislocation density contour plot for the parabolic thermal profile of Eq. (4-8), 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.
FINAL LOCATION DENSITY ALONG THE 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

\( N_0 = 13/\text{cm}^2 \)
\( N_0 = 5/\text{cm}^2 \)
\( N_0 = 1/\text{cm}^2 \)
ADVANCED SILICON SHEET

Dislocation Density Contour Plot

WESTINGHOUSE PROFILE, NO=0.25/CM²×2, R/T=0
UNIT OF X AND Y=CM, Z=1 PER CM××2

LEGEND: Z

- 39
- 774
- 1156
- 1538
- 1920
- 2302
- 2684

- 201
- 583
- 965
- 1347
- 1729
- 2111
- 2493

258
Dislocation Density Contour Plot

WESTINGHOUSE PROFILE. \( \text{Ho} = 0.375 / \text{cm}^2 \)
UNIT OF X AND Y = \text{cm}. \( Z = 1 / \text{cm}^2 \). \( A/T = 1.6667 \) M

LEGEND: \( Z \)

- - - - 130
- - - - 750
- - - - 1370
- - - - 1990
- - - - 2610
- - - - 3230
- - - - 3850
- - - - 4470

Note Low Densities
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Effective Plastic Strain Rate

WESTINGHOUSE PROFILE, NO=0.25/CM*CM
WIDTH = 6 CM, LENGTH = 8 CM, A/T=0.
UNIT OF X AND Y = CM, Z = 10^-5 PER SEC

PLASTIC STRAIN RATE

No indentation

D
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Effective Plastic Strain Rate

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

PLASTIC STRAIN RATE
Residual Stress XX Along Ribbon
Width for Westinghouse Profile

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

RESIDUAL STRESS MPA

Y (CM)
Deflection Shape

WAVELENGTH (C) = 1.0, LENGTH = 8.0
DIAMETER OF DENDRITES IS 0.0 INCHES
CRITICAL THICKNESS = 0.00528 INCHES

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

HALF-WIDTH (C) = 1.0, LENGTH = 8.0
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>=</td>
<td>left, 60' (-120') ✓</td>
<td></td>
</tr>
<tr>
<td>=</td>
<td>=</td>
<td>left, 60' (+120') ✓</td>
<td></td>
</tr>
<tr>
<td>=</td>
<td>=</td>
<td>left, edge</td>
<td></td>
</tr>
<tr>
<td>&lt;0 1 1&gt;</td>
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<td>left, screw</td>
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</tr>
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<tr>
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<td>=</td>
<td>left, edge</td>
<td></td>
</tr>
<tr>
<td>&lt;1 0 -1&gt;</td>
<td>&lt;1 0 -1&gt;</td>
<td>right, screw</td>
<td></td>
</tr>
<tr>
<td>=</td>
<td>=</td>
<td>right, 60' (-120') ✓</td>
<td></td>
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</tr>
<tr>
<td>&lt;0 -1 1&gt;</td>
<td>&lt;0 -1 1&gt;</td>
<td>transv., screw</td>
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<tr>
<td>=</td>
<td>=</td>
<td>transv., 60' (+120') ✓</td>
<td></td>
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<td>=</td>
<td>=</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 3cm/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,

\[ V_0 \] is 0.035 for screw and 0.01 m³/MN·sec for 60'.

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

---

Legend:
- $-2.047885$
- $-0.722240$
- $-0.877795$
- $3.102395$
- $6.777948$

Sign Change: $d_x = \pm 0.125$

Left:
- $(-) \Rightarrow F$
- $(+) \Rightarrow F$

Plot indicates variations in resolved shear stress with specified values.
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Motion of Dislocation

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

possible 60° dislocations emerging to the surface

<table>
<thead>
<tr>
<th>burger's vector</th>
<th>tangent vecto:</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) left strong</td>
<td></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) split</td>
<td></td>
</tr>
<tr>
<td>a/2(0 1 1)</td>
<td>(-1 0 -1)</td>
<td>(-1 -1 1) right weak</td>
<td></td>
</tr>
<tr>
<td>a/2(1 0 -1)</td>
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<td>(-1 0 -1)</td>
<td>(1 -1 -1) left weak</td>
<td></td>
</tr>
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</table>

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

From the K. Sumino's equation of dislocation multiplication

\[ \frac{dN}{dt} = K K_0 N_{m1} (T_a - G b \sqrt{N_{m2}} / \beta)^{m+\lambda} \exp(-Q/kT) dt \quad (A) \]

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

\( N_{m1} \) : dislocation density

\( N_{m1} \alpha \) source density

\( N_{m2} \) 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) \( N_{m1} \) and \( N_{m2} \) are total density of dislocations

(2) \( N_{m1} \) is the partial density of dislocations on each slip system and

\( N_{m2} \) is the total density of dislocations.

(3) Both \( N_{m} \)'s are partial densities of dislocations on each slip system
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Method Calculating Dislocation Density

\[
\begin{array}{ll}
N_{m1} & N_{m2} \\
\hline
\end{array}
\]

1. \( \rightarrow \) \( \text{RSS}_i \) \( \text{total density} = N_{m1} = N_{m2} \)
   \[ dN_m = dN_{m1} = dN_{m2} \]

2. \( \rightarrow \) \( \text{RSS}_i \) \( \text{total density} = \sum_i (N_{m1})_i = N_{m2} \)
   \[ dN_{m2} = \sum_i (dN_m)_i \]

3. \( \rightarrow \) \( \text{RSS}_i \) \( \text{total density} = \sum_i (N_{m1})_i = \sum_i (N_{m2})_i \)
   \[ (dN_{m1})_i = (dN_{m2})_i \]
Total Density of Dislocation Using YI, YTOT and DGEAR

INITIAL TOTAL DENSITY IS 90/MX2 LAMDA IS 1.0

LEGEND: DENS
- 8.5915E+17
- 6.0140E+18
- 3.4366E+19
- 1.1169E+19
- 1.3746E+19

273
Total Density of Dislocation Using Y1, YI and DGEAR

INITIAL TOTAL DENSITY IS 90/M^2. LAMDA IS 1.0
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Averaging the $|\tau_a|$ in Calculating Density

--- liq-sol. interface

$\rightarrow$ liq-sol. interface

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 (1 0 1)</td>
<td>(-1 -1 1)</td>
<td>left</td>
</tr>
<tr>
<td>a/2 (0 1 1)</td>
<td>(-1 -1 1)</td>
<td>left</td>
</tr>
<tr>
<td>a/2 (-1 1 0)</td>
<td>(-1 -1 1)</td>
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<tr>
<td>a/2 (1 0 -1)</td>
<td>(-1 1 -1)</td>
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<tr>
<td>a/2 (1 1 0)</td>
<td>(-1 1 -1)</td>
<td>right</td>
</tr>
<tr>
<td>a/2 (0 1 1)</td>
<td>(-1 1 -1)</td>
<td>right</td>
</tr>
<tr>
<td>a/2 (0 -1 1)</td>
<td>(1 -1 -1)</td>
<td>transverse</td>
</tr>
<tr>
<td>a/2 (1 0 1)</td>
<td>(1 -1 -1)</td>
<td>transverse</td>
</tr>
<tr>
<td>a/2 (1 1 0)</td>
<td>(1 -1 -1)</td>
<td>transverse</td>
</tr>
</tbody>
</table>
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Density of Dislocations When NO is 1 at \( x = 0.2 \text{ cm} \)

\[ \text{UNIT OF X IS CM, Z IS DENSITY IN } 1/\text{M}^2 \]
Density of Dislocations When NO is 1 at x = 0.2 cm

UNIT OF X IS CM, Z IS DENSITY IN 1/M**2
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Density of Dislocations When NO is 1 at x = 0.2 cm

UNIT OF X IS CM, Z IS DENSITY IN 1/M**2
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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>
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<td>[011] [111] R</td>
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</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.
Dislocation Distribution in Web Dendrite Ribbon

(a) Top View of Etched Web Ribbon

(b) Dislocation distribution

(c) Magnified view with 30° orientation

100 microns
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Cz Temperature Dependence

![Graph showing Cz Temperature Dependence](image)

Cz Strain Rate Dependence

![Graph showing Cz Strain Rate Dependence](image)
ADVANCED SILICON SHEET

Cz Temperature Dependence

Web Ribbon: Strain Rate Dependence
Web Ribbon: Temperature Dependence

![Graph showing temperature dependence of R.S. stress vs. 1000/T (°C⁻¹)]

- **Strain Rate = 1e-04**
- **Strain Rate = 1e-05**

Equation:

\[ S_{\text{strain}} \cdot N = 2 \times 10^4 \text{ m}^{-1} \]

\[ S = 1.2 \times 10^{-5} \text{ sec} \]