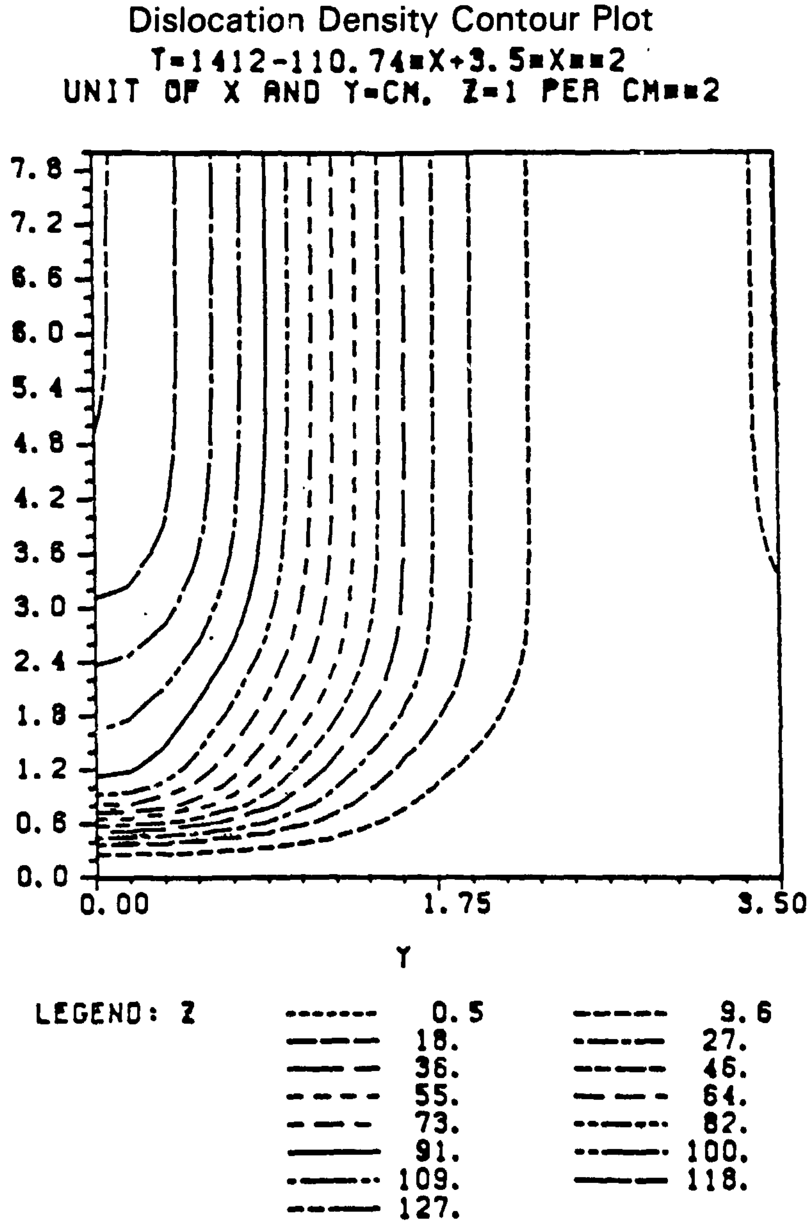
N87-16408

ANALYSIS OF SILICON STRESS/STRAIN RELATIONSHIPS

UNIVERSITY OF KENTUCKY

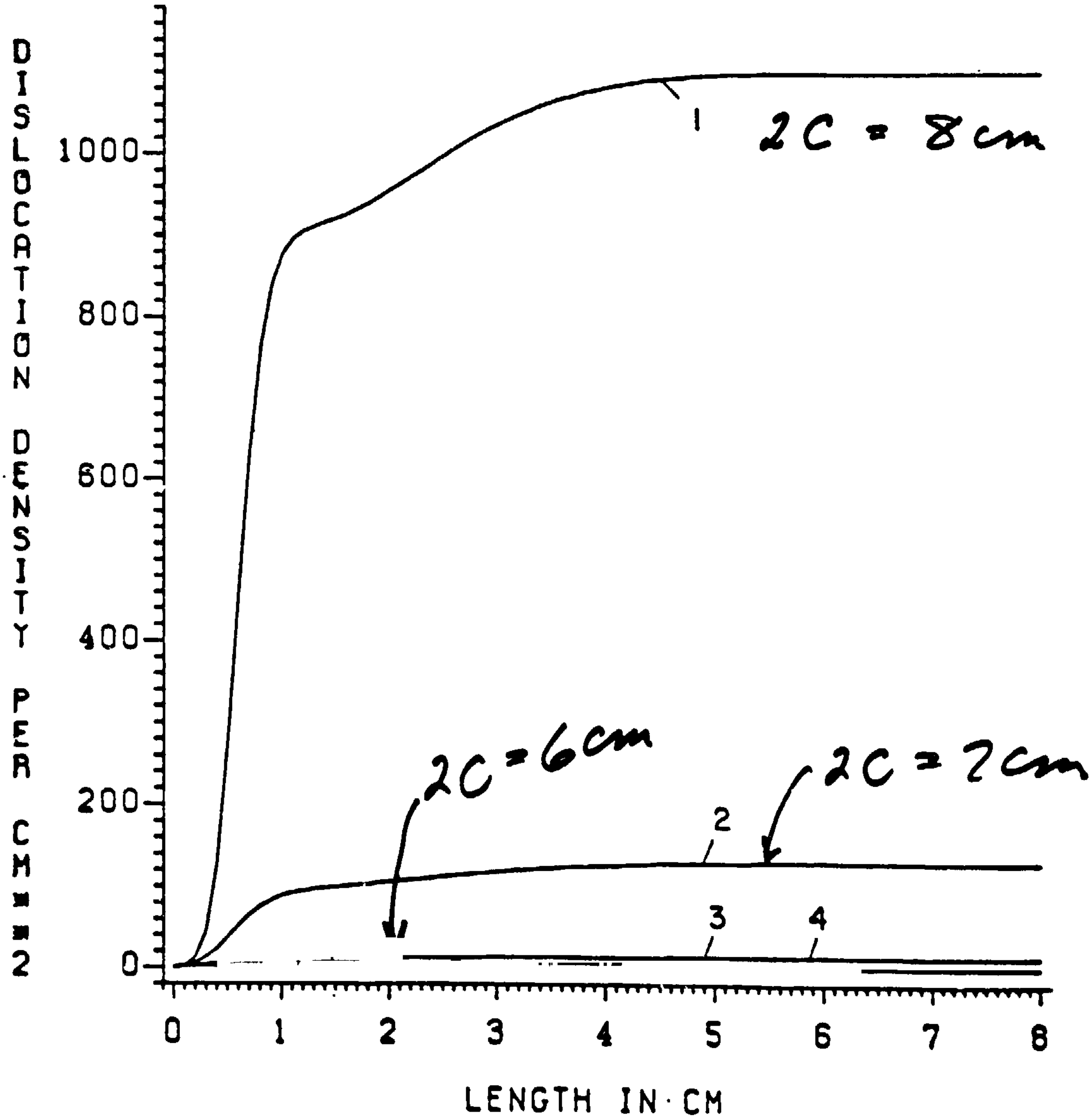
O. Dillon



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}.

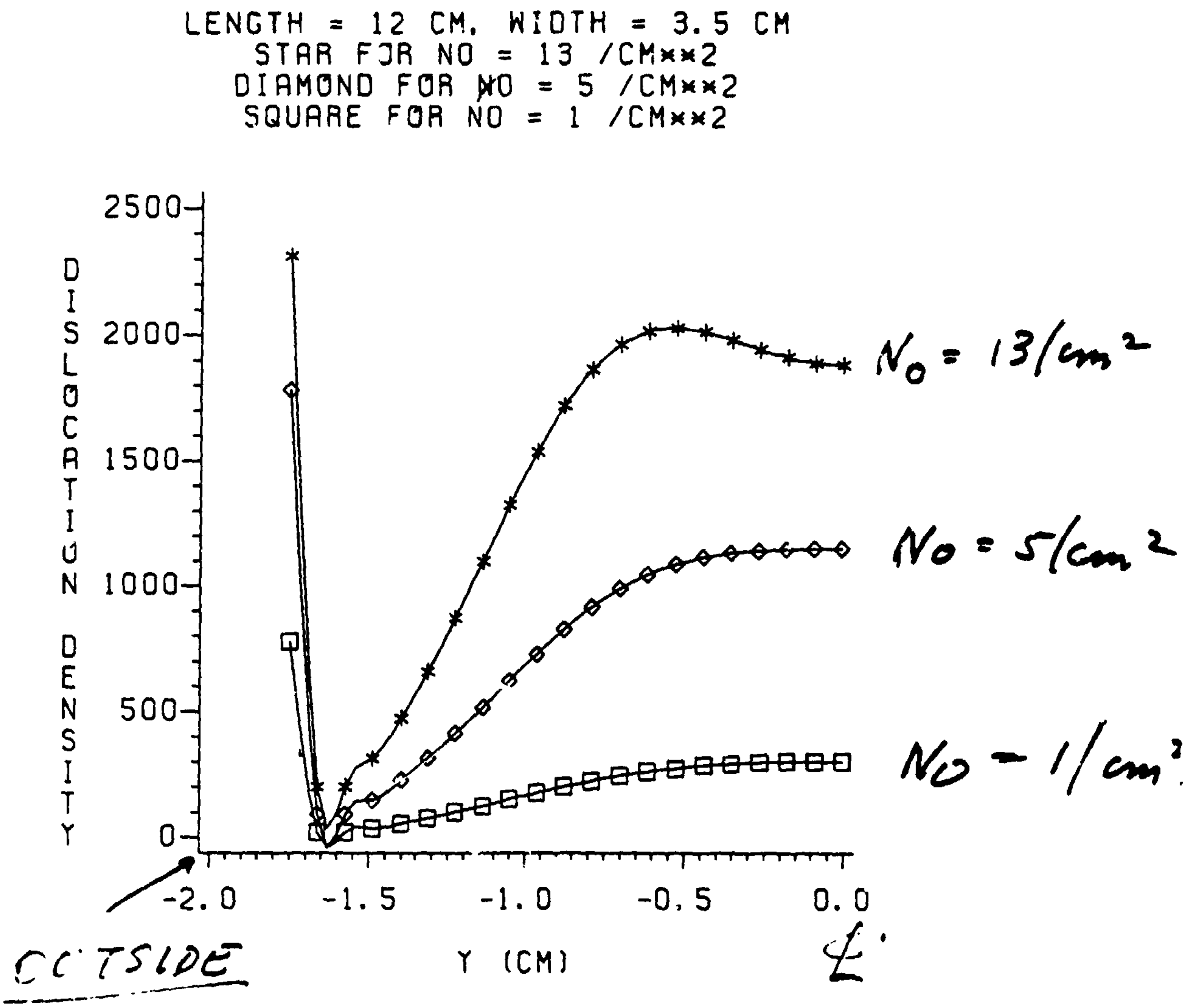
Dislocation Density Along Y = 0 (Centerline)
T=1412-110.74*X+3.5*X**2

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

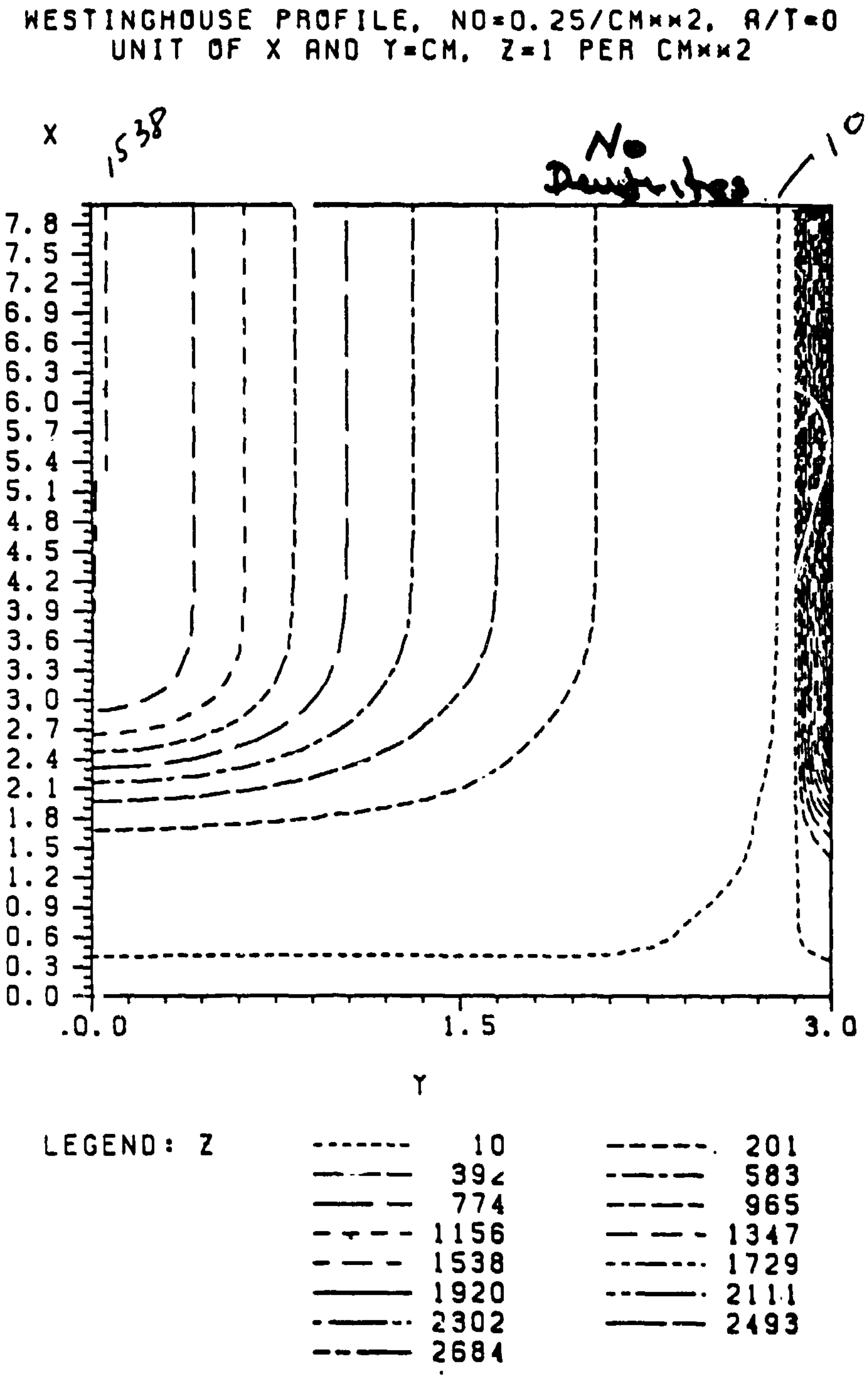


Dislocation density along the centerline of the ribbon for the parabolic thermal profile of Eq. (4-8), initial dislocation density = 0.5 cm^{-2}, and width = 8, 7, 6, 4 cm.

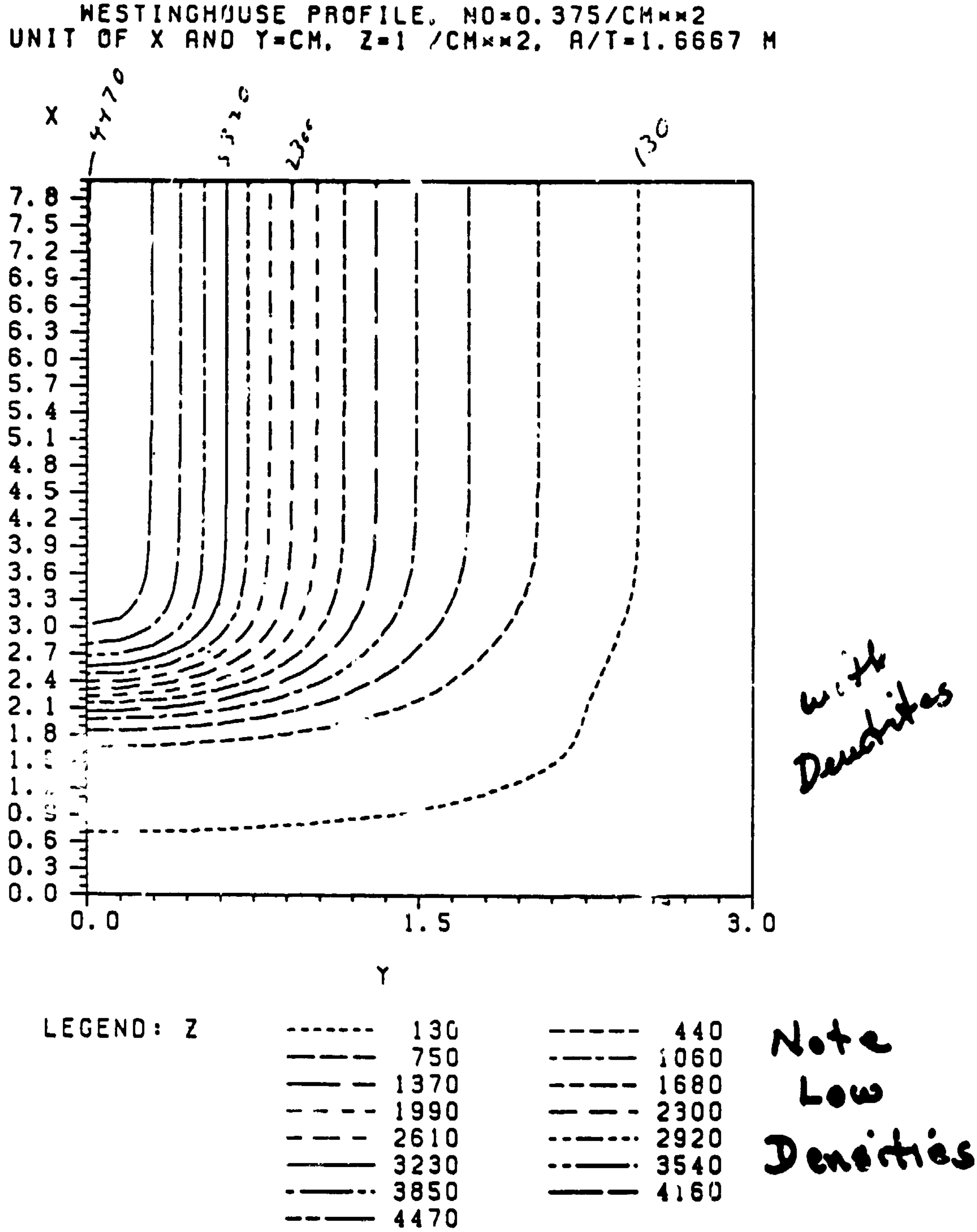
Final Dislocation Density Along the Ribbon Width for Westinghouse Profile



Dislocation Density Contour Plot

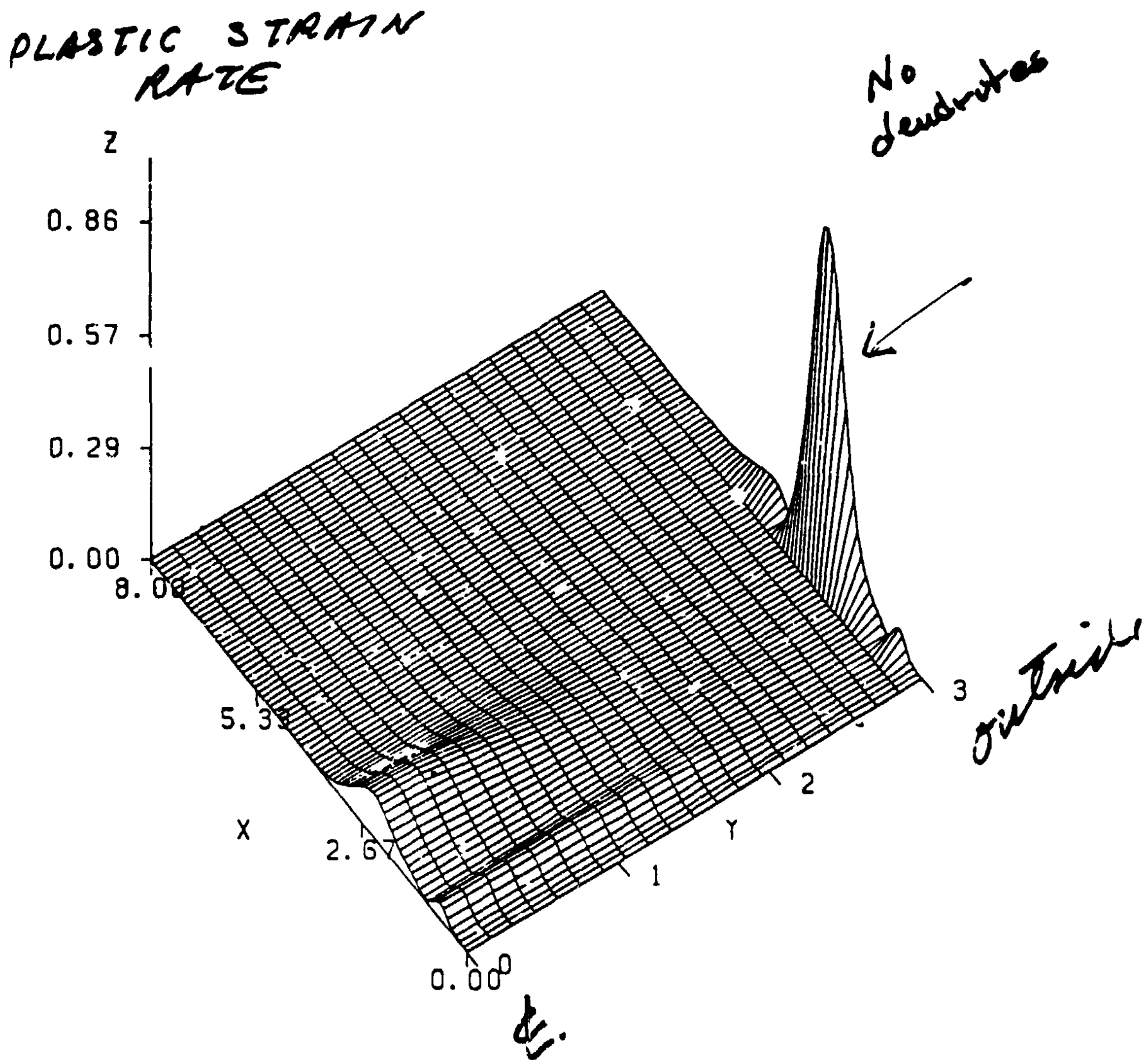


Dislocation Density Contour Plot



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



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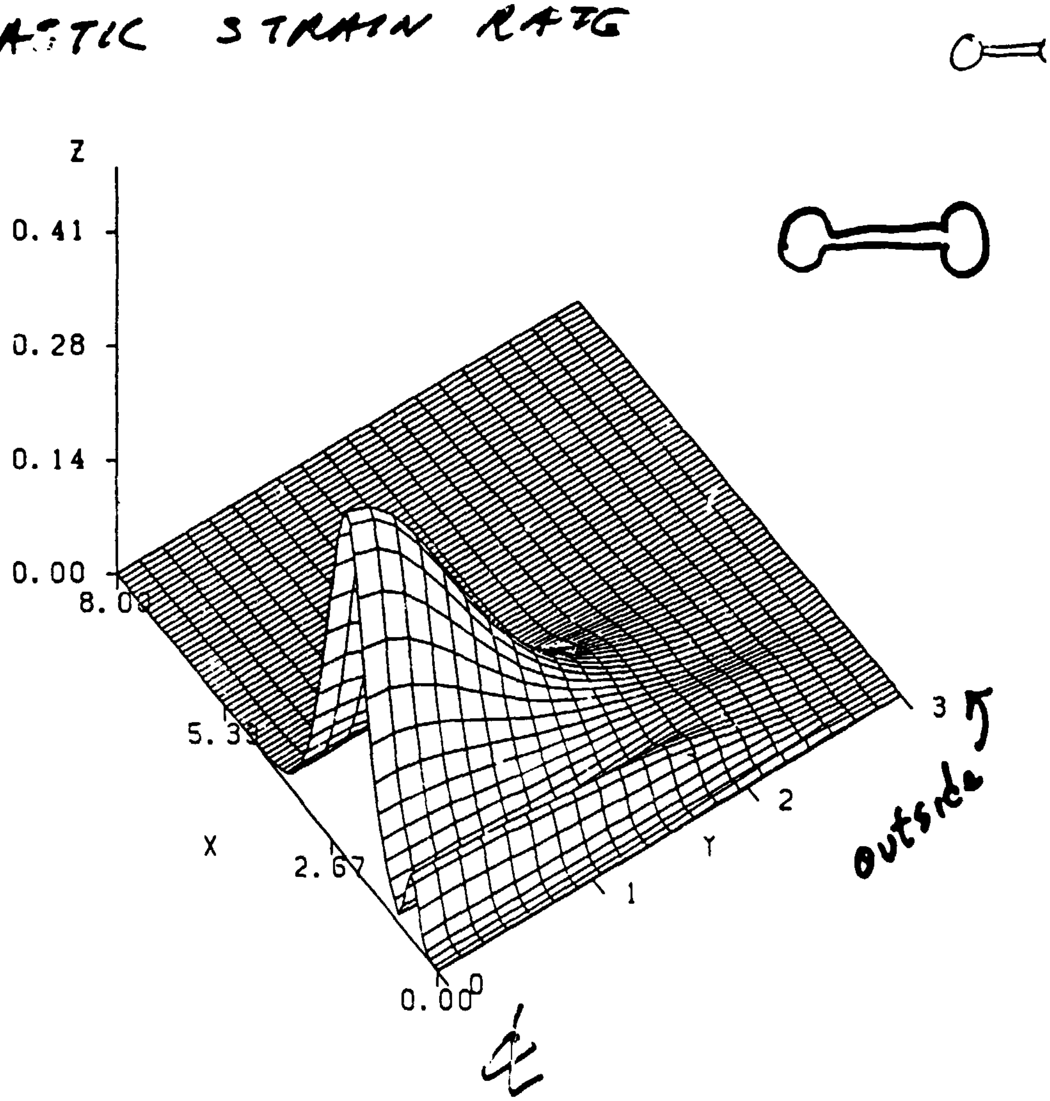
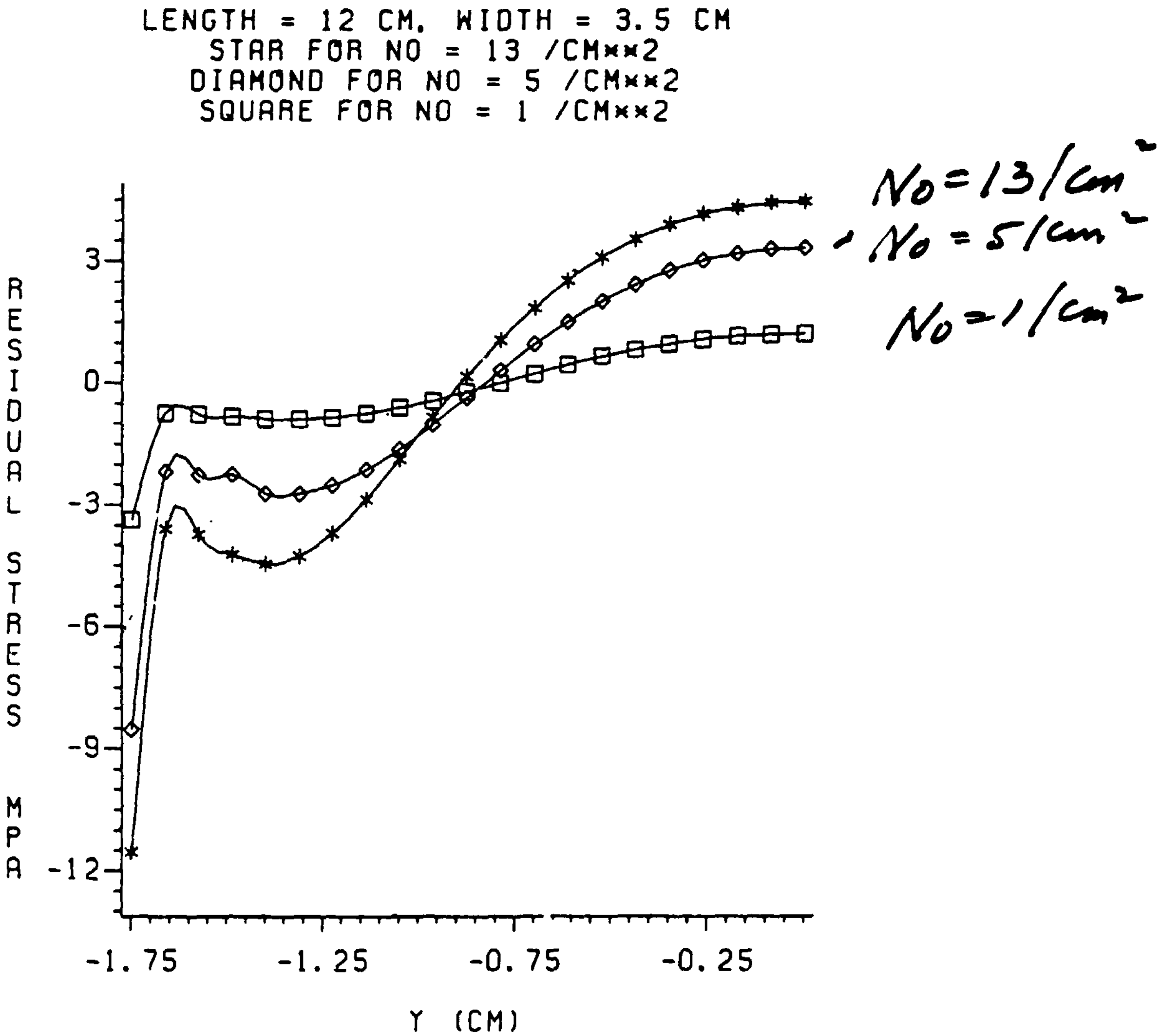
Effective Plastic Strain Rate

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



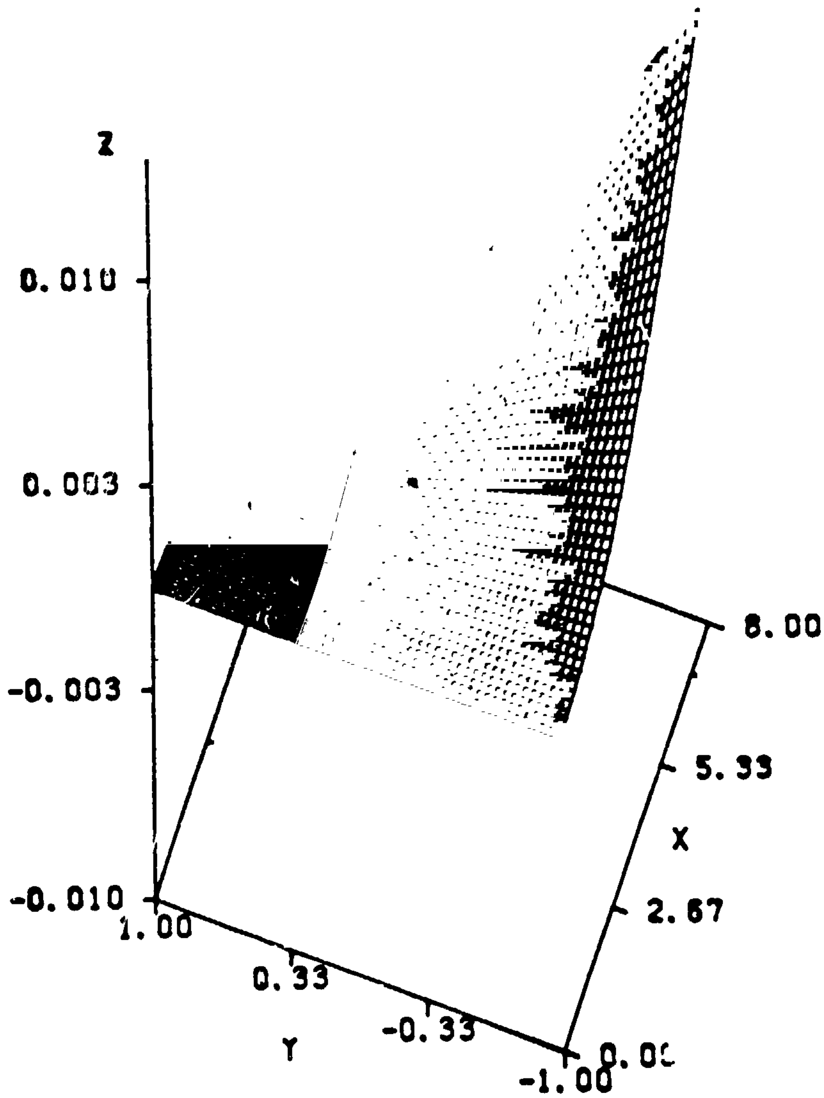
Residual Stress XX Along Ribbon
Width for Westinghouse Profile



Deflection Shape

HALF-WIDTH (C)=1., LENGTH=8.0
DIAMETER OF DENDRITES IS 0.0 INCHES
CRITICAL THICKNESS = 0.00526 INCHES

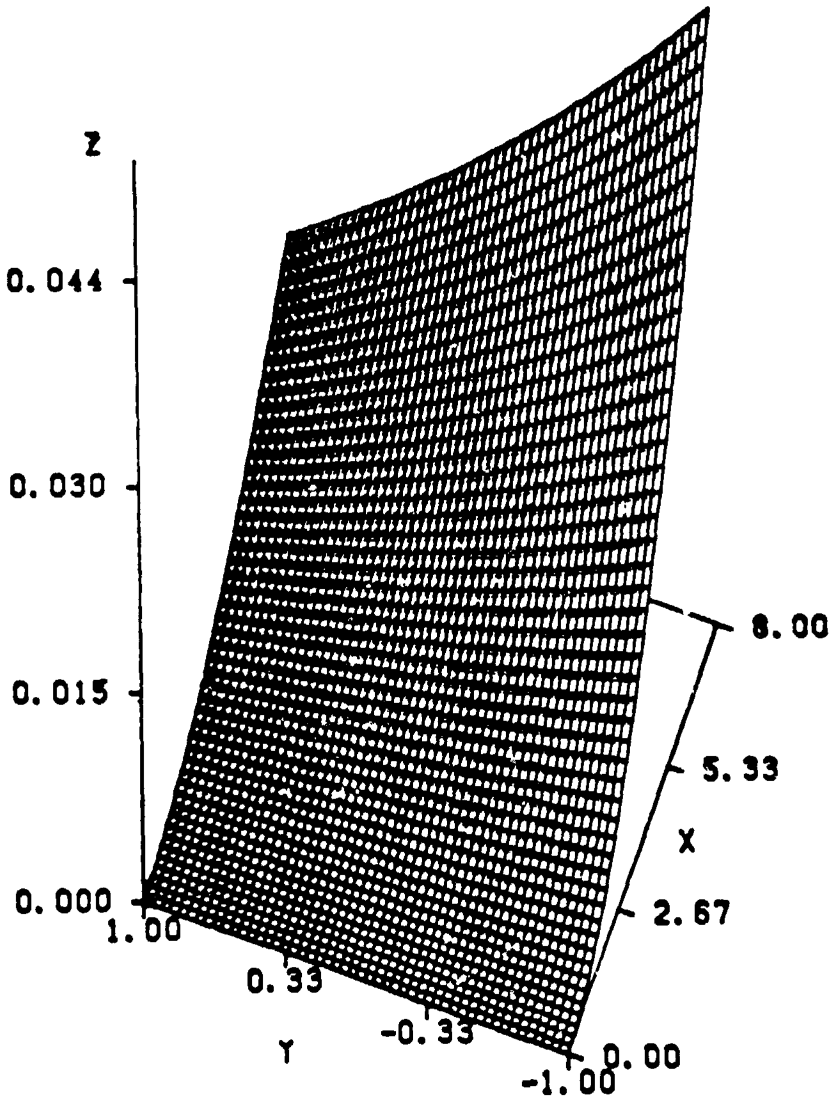
T(x) = parabolic



Deflection Shape

HALF-WIDTH (C)=1., LENGTH=8.0
DIAMETER OF DENDRITES IS 0.2 INCHES
CRITICAL THICKNESS = 0.057120 INCHES

$T(x) =$ 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

burgers vector	tangent vector	slip plane	type of dislocation
<-1 0 -1>	<-1 0 -1>	(-1 -1 1),left,	screw
=	<0 1 1>	= ,left,	60' (-120') ✓
=	<1 -1 0>	= ,left,	60' (+120')
=	<1 -2 -1>	= ,left,	edge
<0 1 1>	<0 1 1>	= ,left,	screw
=	<1 -1 0>	= ,left,	60' (+120')
=	<-1 0 -1>	= ,left,	60' (-120') ✓
=	<-2 1 -1>	= ,left,	edge
<-1 1 0>	<-1 1 0>	= ,left,	screw
=	<0 -1 -1>	= ,left,	60' (-120') ✓
=	<1 0 1>	= ,left,	60' (+120') ✓
=	<-1 -1 2>	= ,left,	edge
<1 0 -1>	<1 0 -1>	(-1 1 -1),right,	screw
=	<-1 -1 0>	= ,right,	60' (-120') ✓
=	<0 1 1>	= ,right,	60' (+120') ✓
=	<-1 -2-1>	= ,right,	edge
<0 -1 -1>	<0 -1 -1>	= ,right,	screw
=	<1 1 0>	= ,right,	60' (-120') ✓
=	<-1 0 1>	= ,right,	60' (+120')
=	<-2 -1 1>	= ,right,	edge
<1 1 0>	<1 1 0>	= ,right,	screw
=	<-1 0 1>	= ,right,	60' (+120')
=	<0 -1 -1>	= ,right,	60' (-120') ✓
=	<-1 1 -2>	= ,right,	edge
<0 -1 1>	<0 -1 1>	(-1 1 -1),transv.,	screw
=	<1 1 0>	= ,transv.,	60' (+120') ✓
=	<-1 0 -1>	= ,transv.,	60' (-120') ✓
=	<2 1 1>	= ,transv.,	edge
<1 1 0>	<1 1 0>	= ,transv.,	screw
=	<0 -1 1>	= ,transv.,	60' (+120')
=	<-1 0 -1>	= ,transv.,	60' (-120') ✓
=	<1 -1 2>	= ,transv.,	edge
<1 0 1>	<1 0 1>	= ,transv.,	screw
=	<-1 -1 0>	= ,transv.,	60' (-120') ✓
=	<0 1 -1>	= ,transv.,	60' (+120')
=	<-1 -2 1>	= ,transv.,	edge

(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 burger's 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

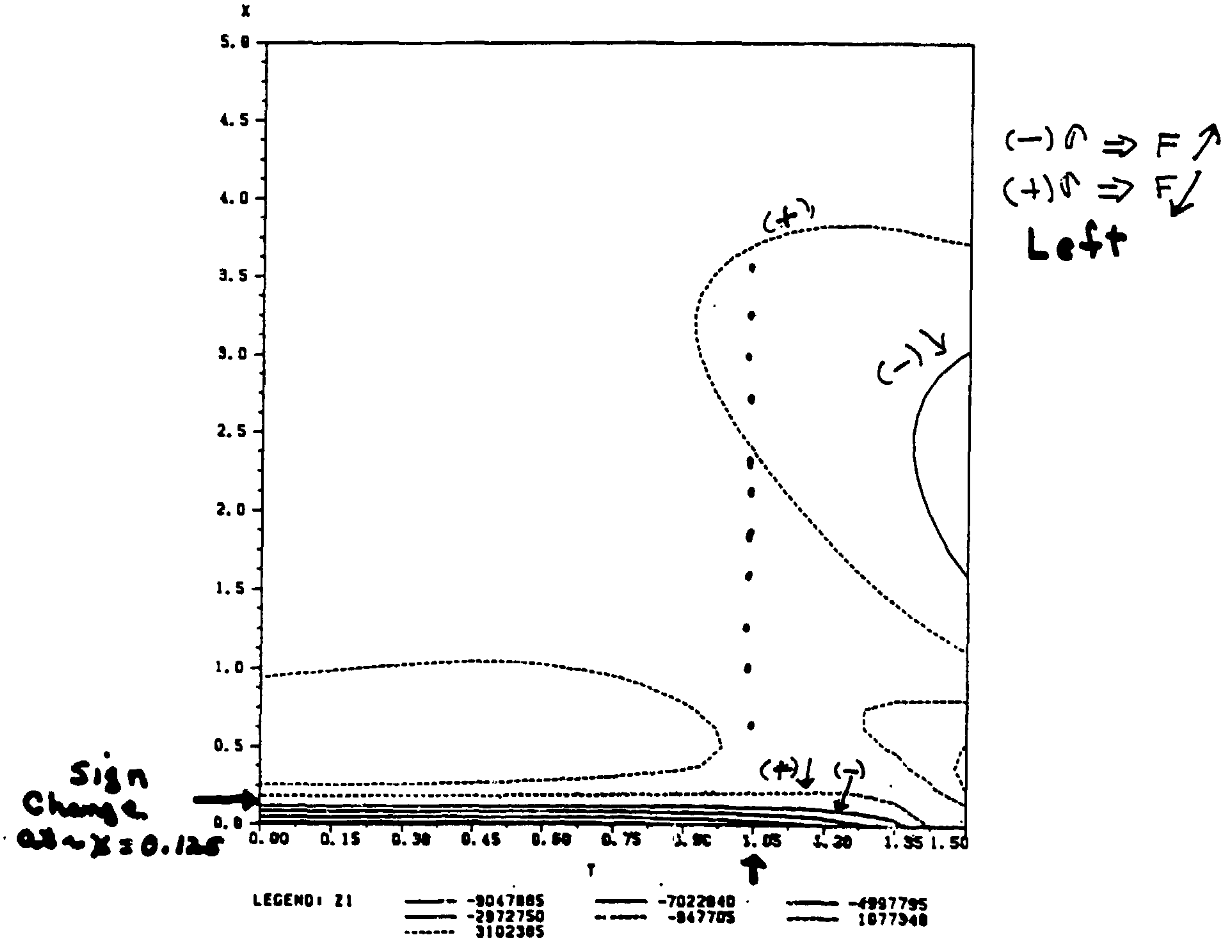
$$V = V_0 \tau \exp(-E/kT)$$

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

V_0 is 0.035 for screw and 0.01 m^3 / MN.sec for 60'.

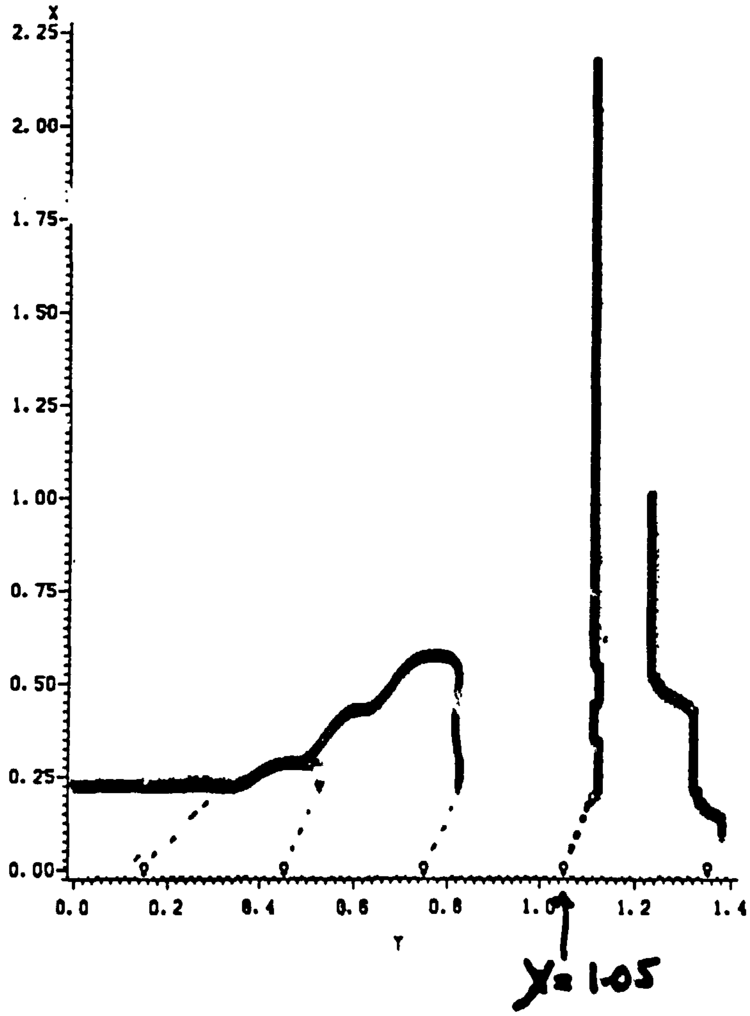
is still valid at high temperature like around melting temperature.

Resolved Shear Stress



Motion of Dislocation

B=A/2(-1 1 0),T=(1 0 1),N=(-1 -1 1)



UNIT OF AXES ARE CM

Motion of the Dislocations Emerging to the Surface

possible 60' dislocations emerging to the surface

burger's vector	tangent vecto:	plane	motion
a/2(-1 0 -1)	(0 1 1)	(-1 -1 1)	left strong
a/2(-1 1 0)	(0 -1 -1)	(-1 -1 1)	*
a/2(-1 1 0)	(1 0 1)	(-1 -1 1)	split
a/2(0 1 1)	(-1 0 -1)	(-1 -1 1)	right weak
a/2(1 0 -1)	(0 1 1)	(-1 1 -1)	right strong
a/2(1 0 -1)	(-1 -1 0)	(-1 1 -1)	*
a/2(1 1 0)	(0 -1 -1)	(-1 1 -1)	*
a/2(0 -1 -1)	(1 1 0)	(-1 1 -1)	right weak
a/2(0 -1 1)	(-1 0 -1)	(1 -1 -1)	right strong
a/2(0 -1 1)	(-1 -1 0)	(1 -1 -1)	left strong
a/2(1 0 1)	(-1 -1 0)	(1 -1 -1)	left weak
a/2(1 1 0)	(-1 0 -1)	(1 -1 -1)	left weak

* ; These are forced into the liquid

Calculation of the Density of Dislocations

From the K. Sumino's equation of dislocation multiplication

$$dNm = K\ Ko\ Nm1\ (Ta - G\ b\ SQRT(Nm2)/\beta)^{(m+\lambda)}\ \exp(-Q/kT)\ dt \quad \text{---(A)}$$

where K,Ko,b, β ,m, λ ,k,Q are constants given by K.Sumino

Nm's ; dislocation density

Nm1 α source density

Nm2 is the density controlling the back stress

Ta ; applied stresses

T ; temperature

G ; shear modulus

t ; time

Three possible ways of application of the equation (A)

(1) Nm1 and Nm2 are total density of dislocations

(2) Nm1 is the partial density of dislocations on each slip system and

Nm2 is the total density of dislocaitons

(3) Both Nm's are partial densities of disloations on each slip system

Method Calculating Dislocation Density

Nm_1	Nm_2

(1) $\perp \text{->} RSS_i$ $\perp\perp\perp$ total density $= Nm_1 = Nm_2$

$$dNm = dNm_1 = dNm_2$$

(2) $\perp \text{->} RSS_i$ $\perp\perp\perp$ total density $= \sum_{1}^{9} (Nm_1)_i = Nm_2$

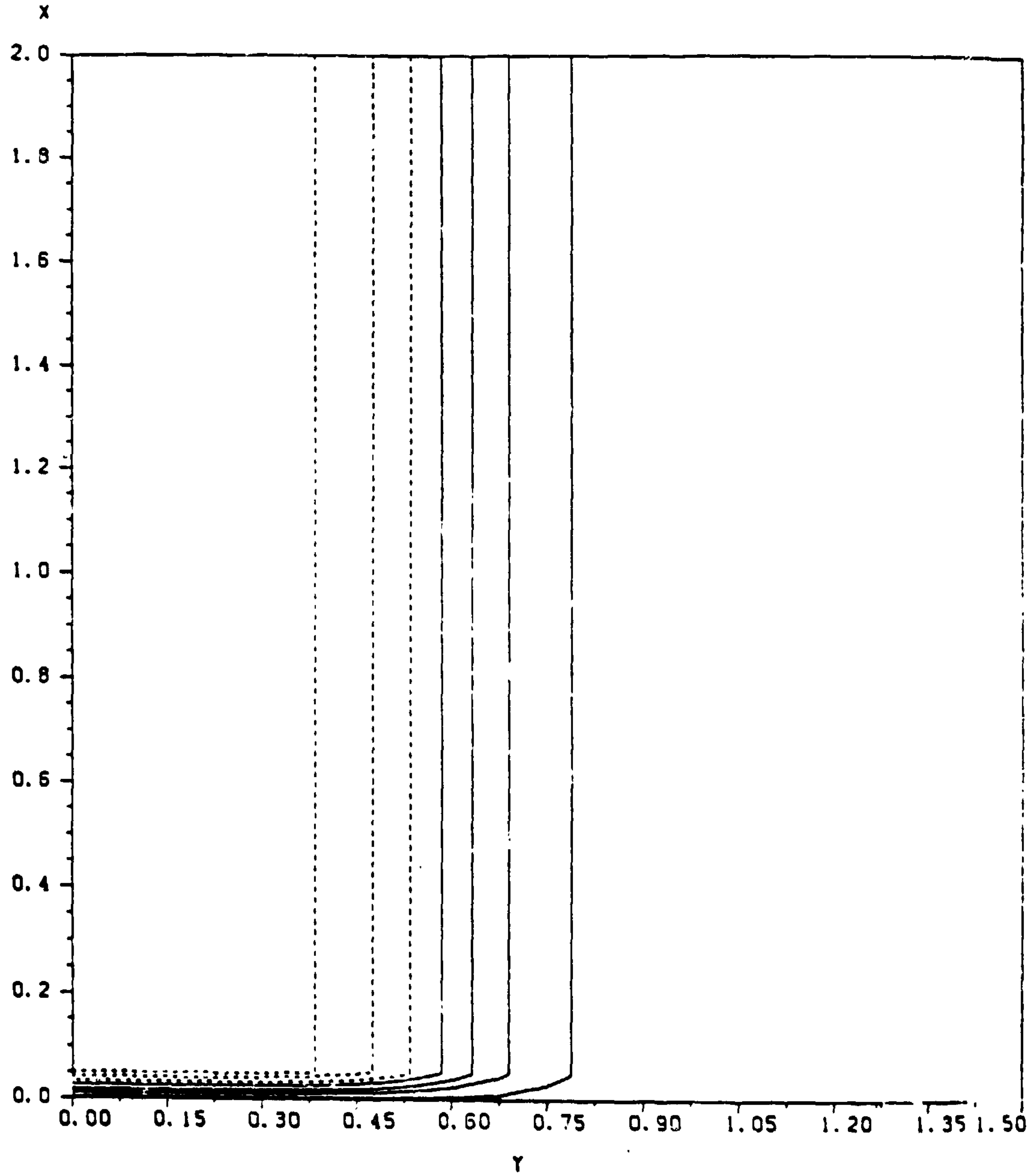
$$dNm_2 = \sum_{1}^{9} (dNm)_i$$

(3) $\perp \text{->} RSS_i$ $\perp\perp\perp$ total density $= \sum_{1}^{9} (Nm_1)_i = \sum_{1}^{9} (Nm_2)_i$

$$(dNm_1)_i = (dNm_2)_i$$

Total Density of Dislocation Using YI, YTOT and DGEAR

INITIAL TOTAL DENSITY IS 90/M**2 LAMDA IS 1.0

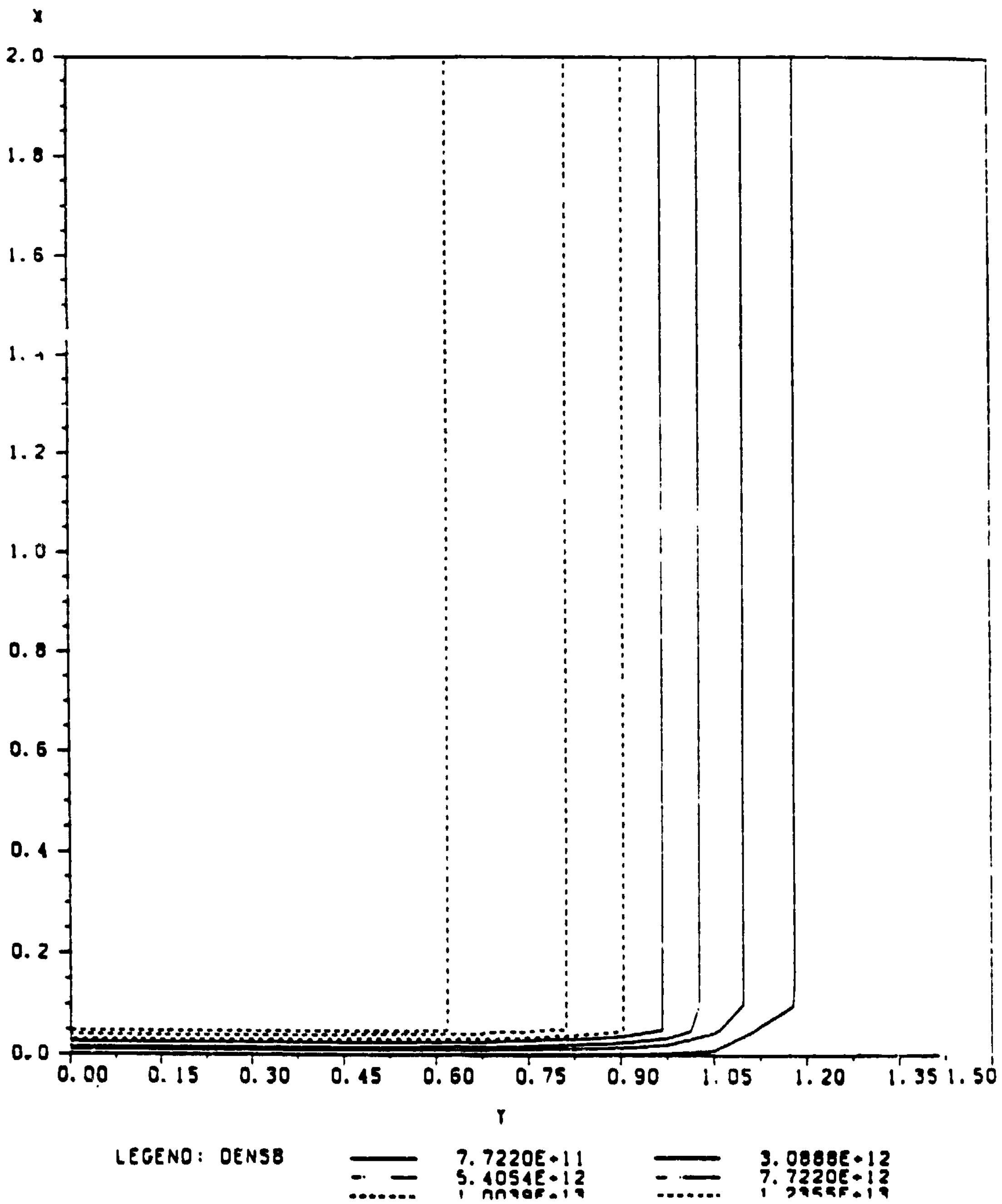


LEGEND: DENS

8.5915E+17	5.4366E+18
6.0143E+18	8.5915E+18
1.1169E+19	1.3746E+19
1.6324E+19	

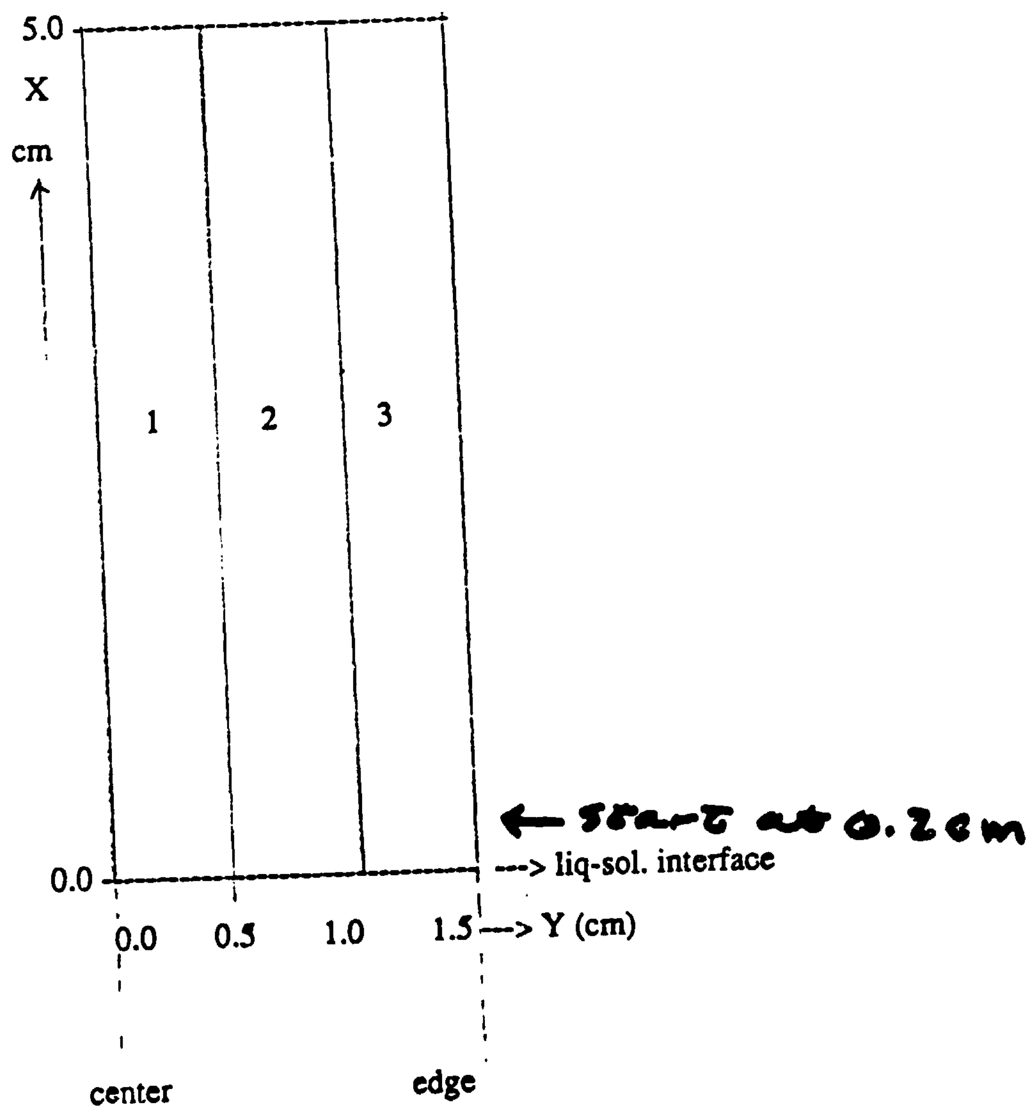
Total Density of Dislocation Using YI, YI and DGEAR

INITIAL TOTAL DENSITY IS 90/M**2 ,LAMDA IS 1.0



C-4

Averaging the $|\tau a|$ in Calculating Density

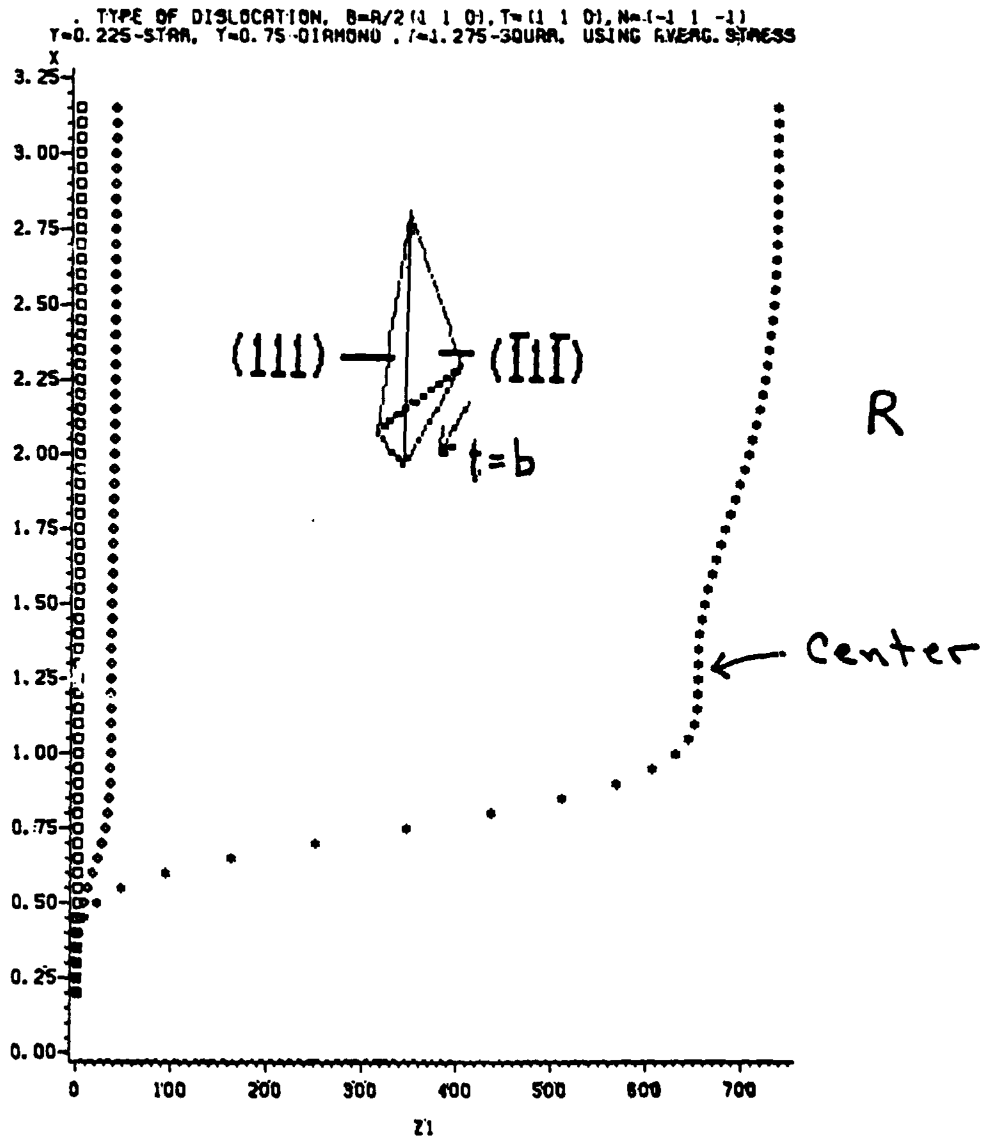


column 1 ; * ,column 2 ;, ♦ column 3 ; □

Nine Slip Systems

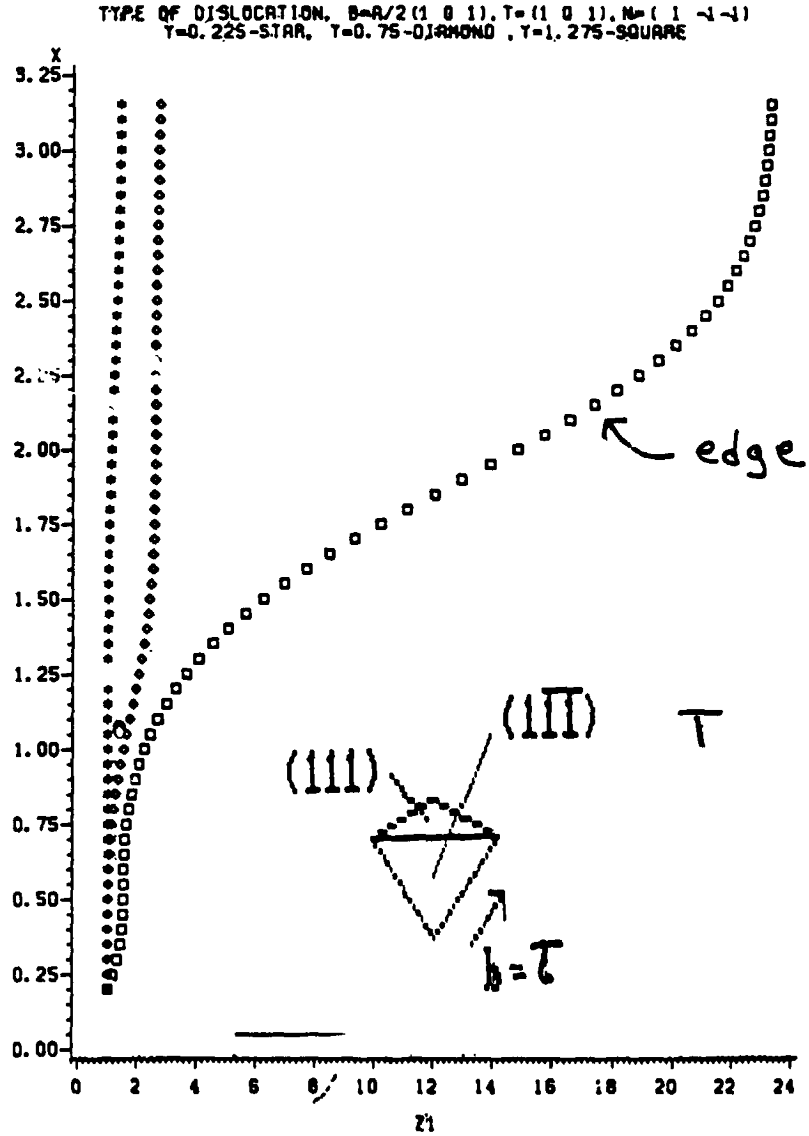
burger's vector	slip plane	type of plane
a/2 (1 0 1)	(-1 -1 1)	left
a/2 (0 1 1)	(-1 -1 1)	left
a/2 (-1 1 0)	(-1 -1 1)	left
a/2 (1 0 -1)	(-1 1 -1)	right
a/2 (1 1 0)	(-1 1 -1)	right
a/2 (0 1 1)	(-1 1 -1)	right
a/2 (0 -1 1)	(1 -1 -1)	transverse
a/2 (1 0 1)	(1 -1 -1)	transverse
a/2 (1 1 0)	(1 -1 -1)	transverse

Density of Dislocations When NO is 1 at x = 0.2 cm



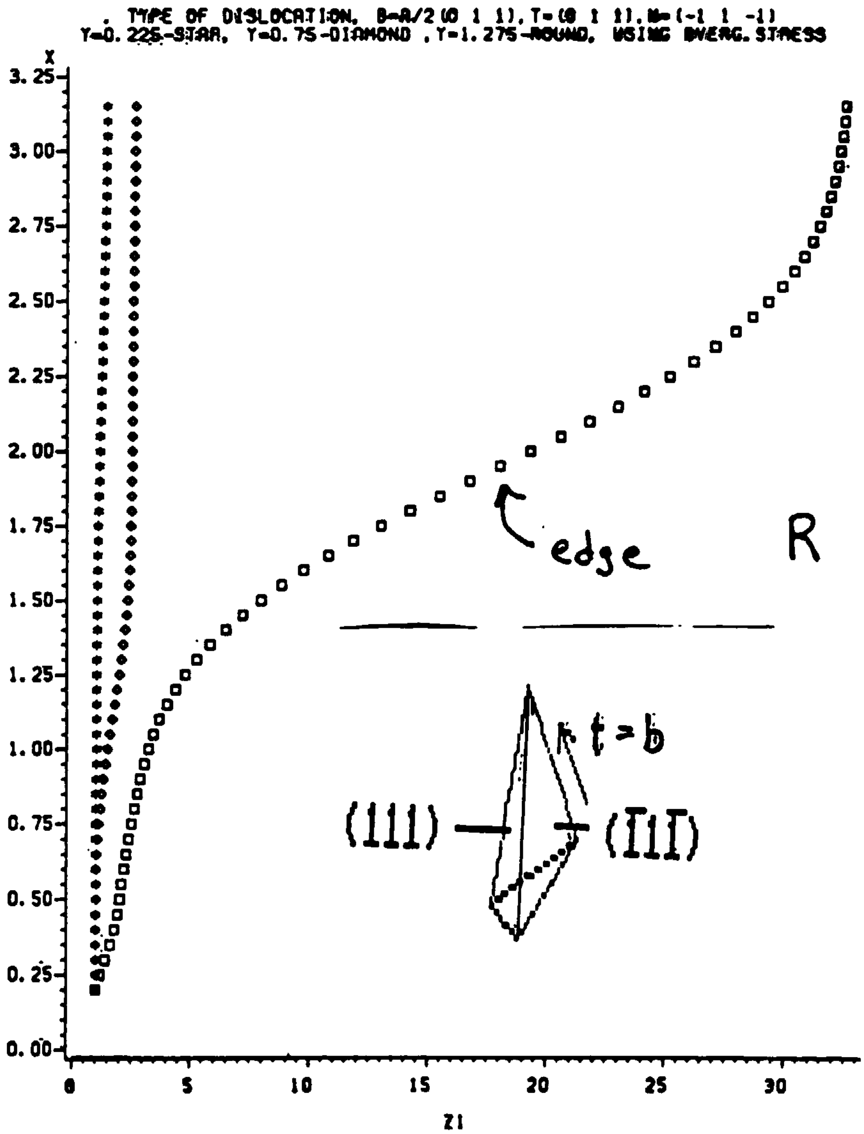
*UNIT OF X IS CM, Z IS DENSITY IN 1/M**2*

Density of Dislocations When NO is 1 at x = 0.2 cm



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

Density of Dislocations When NO is 1 at x = 0.2 cm

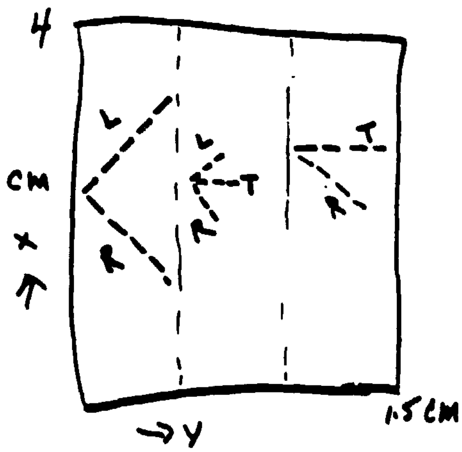


*UNIT OF X IS CM, Z IS DENSITY IN 1/M**2*

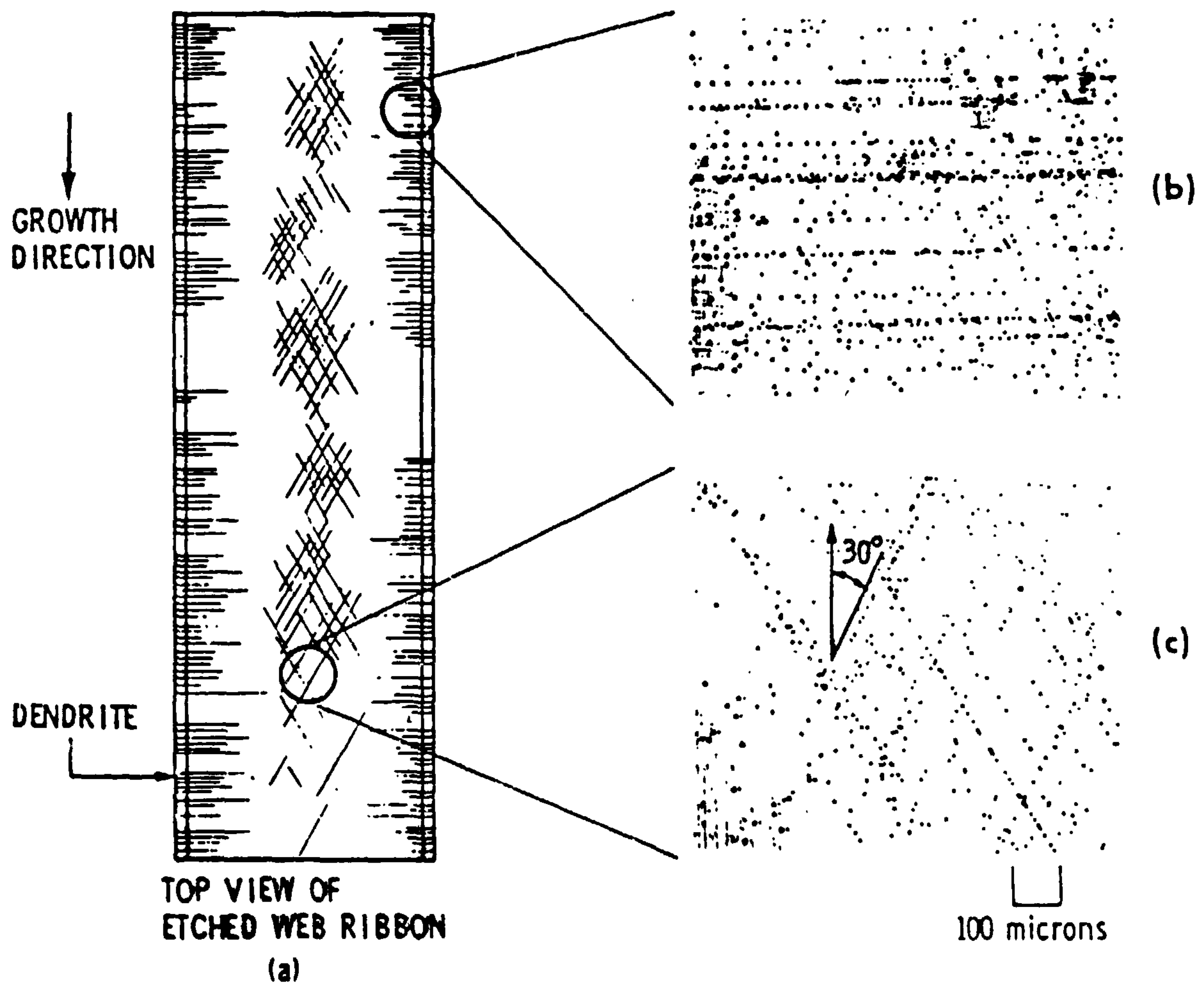
Dislocation Multiplication by Stress Averaging Over 0.5 cm

Dislocation Type			Multiplication Factor		
b	N	Type	Center	Mid-Width	Edge
[101]	[$\bar{1}\bar{1}1$]	L	750	50	1
[011]	[$\bar{1}\bar{1}1$]	L	2.5	3.5	5
[110]	[$\bar{1}11$]	L	23	1	2
[110]	[$\bar{1}1\bar{1}$]	R	750	50	1
[101]	[$\bar{1}1\bar{1}$]	R	12	1	50
[011]	[$\bar{1}1\bar{1}$]	R	1	2.5	35
[101]	[$1\bar{1}\bar{1}$]	T	1	3	24
[110]	[$\bar{1}11$]	T	2	3	10
[011]	[$1\bar{1}\bar{1}$]	T	1.5	66	37

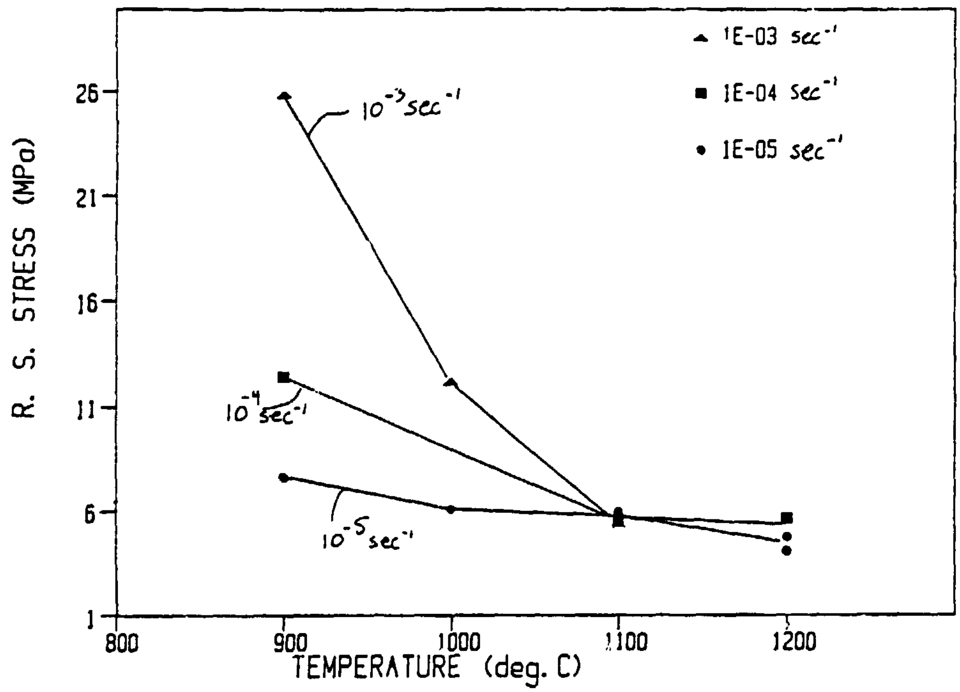
Caiculations started at x=0.2 cm.



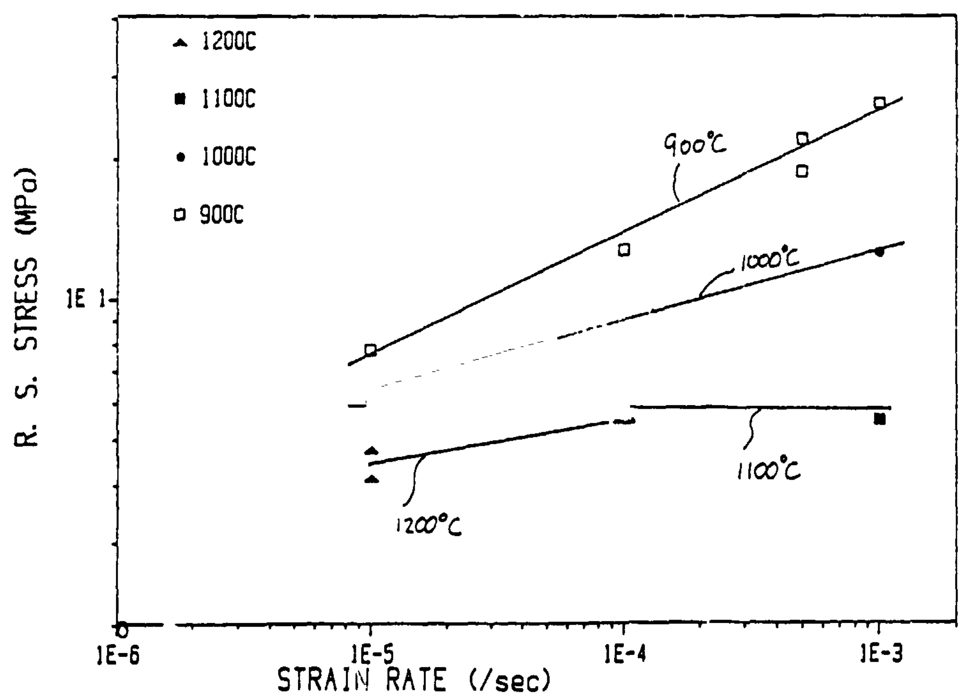
Dislocation Distribution in Web Dendrite Ribbon



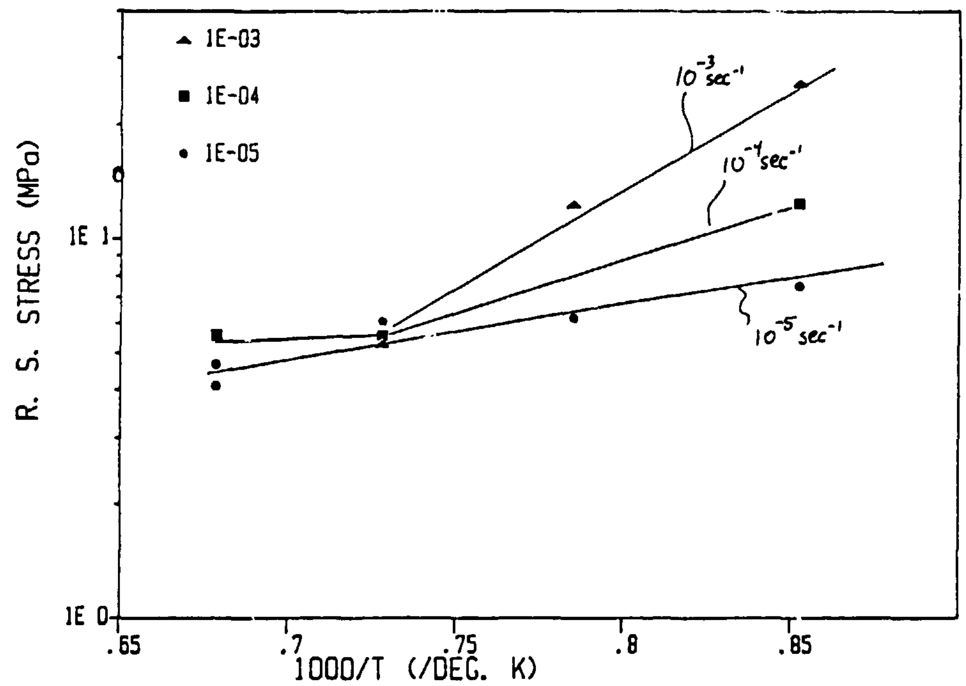
Cz Temperature Dependence



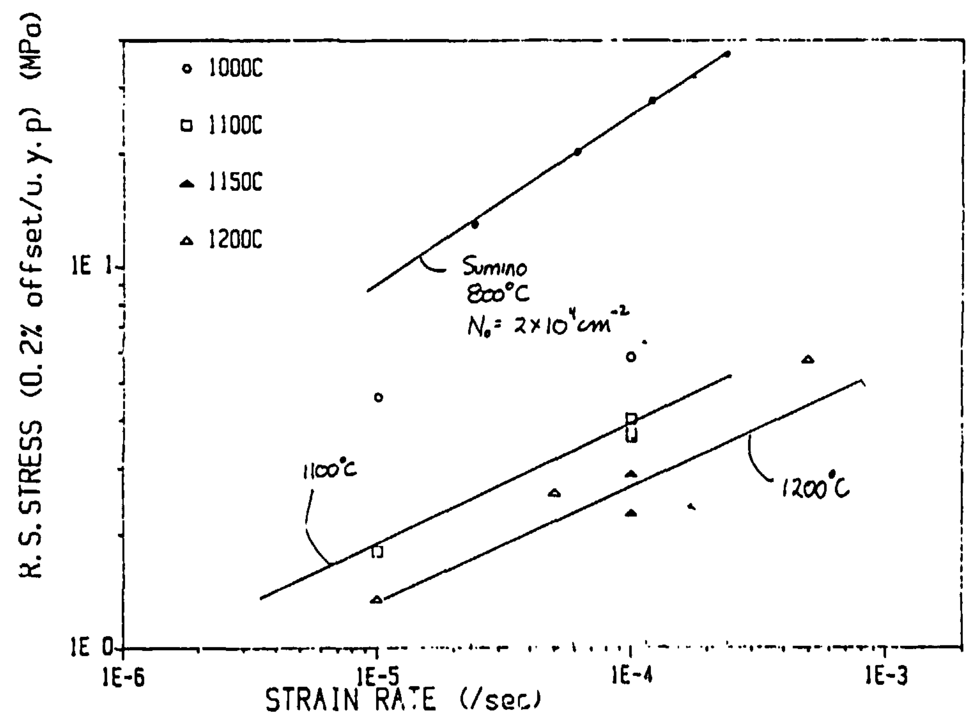
Cz Strain Rate Dependence



Cz Temperature Dependence



Web Ribbon: Strain Rate Dependence



Web Ribbon: Temperature Dependence