Literature Review Examination

Dynamic Behavior of BCC Metals

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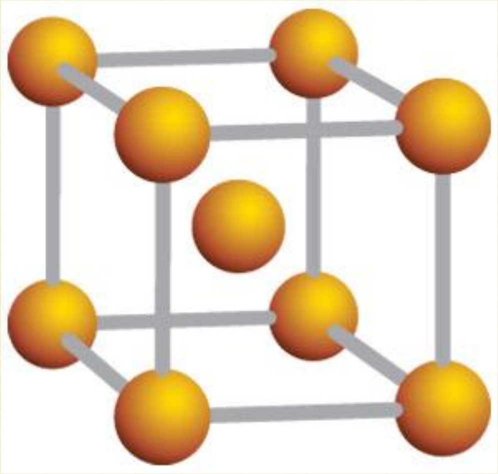
Outline

- Background
- Dynamic Behavior
  - Dislocation motion
  - Mechanical Twinning
  - Grain Size Effects
  - Impurity Effects
- Shock-Wave Deformation
- Summary and Conclusions

Background

BCC Metals



- Some important Body-Centered Cubic (BCC) metals:
  - Iron (Fe): Engineering materials
  - Tungsten (W): High hardness, Electrical conductor
  - Molybdenum (Mo): Withstands extreme temperature
  - Niobium (Nb): Superconducting magnets, Superalloys
  - Tantalum (Ta): Electronic components, Superalloys
  - Vanadium (V): Alloys
  - Chromium (Cr): Corrosion resistance

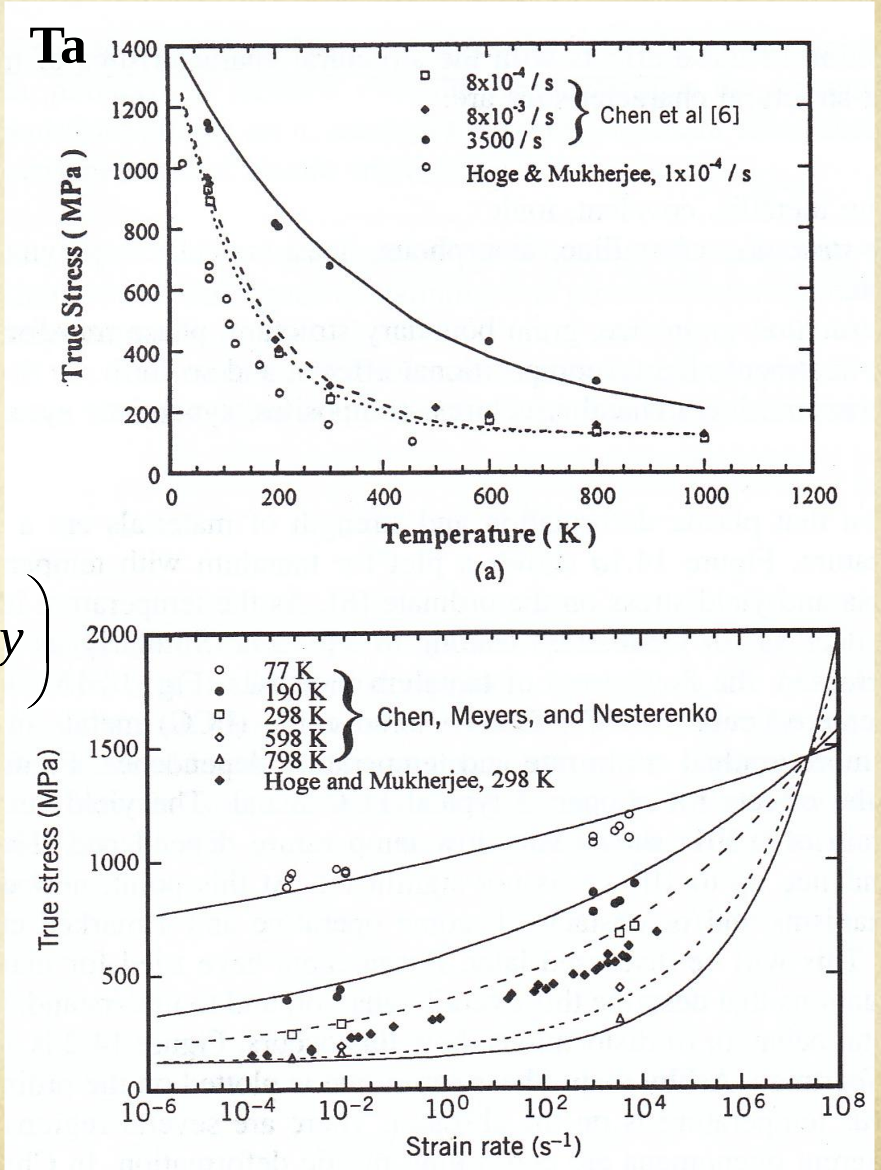
Reference: http://en.wikipedia.org/wiki/Main_Page

BCC Metal Properties

- Plastic deformation and strength of materials are
  - Function of temperature.
  - Function of strain rate.
  - Irreversible processes that are path-dependent
- Objective: constitutive equation

$$\sigma = f\left(P,\ \ \varepsilon,\ \ \frac{d\varepsilon}{dt},\ \ T,\ \ deformation\ \ history \right)$$

- BCC metals: much higher temperature and strain-rate sensitivity than the FCC metals



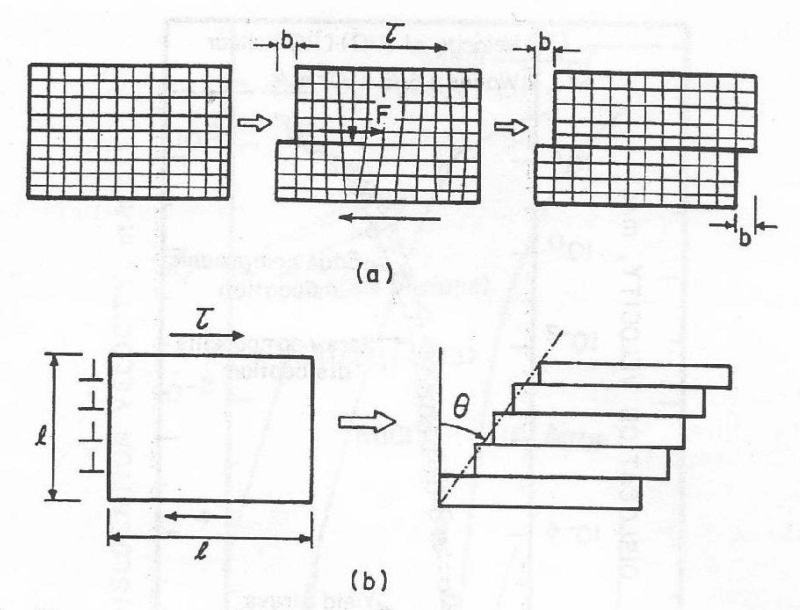
M. A. Meyers, Y. -J. Chen, F. D. S. Marquis, and D. S. Kim, Met. Trans. 26A, (1995) 2493
K. G Hoge and A. K. Mukherjee, J. Matls. Sci. 12 (1977) 1666

Dynamic Behavior

Physical Based Constitutive Equations

- Material responds to external tractions by
  - Dislocation generation and motion

    (most important carriers of plastic deformation in metals)
  - Mechanical twinning
  - Phase transformation
  - Fracture (microcracking, failure, delamination)
  - Viscous glide of polymer chains and shear zones in glasses



- Orowan Equation

$$\gamma = \tan\theta = \frac{Nb}{\ell} = \frac{Nb\ell}{\ell^2} = \rho b \ell$$

$$\dot{\gamma} = \rho b \upsilon$$

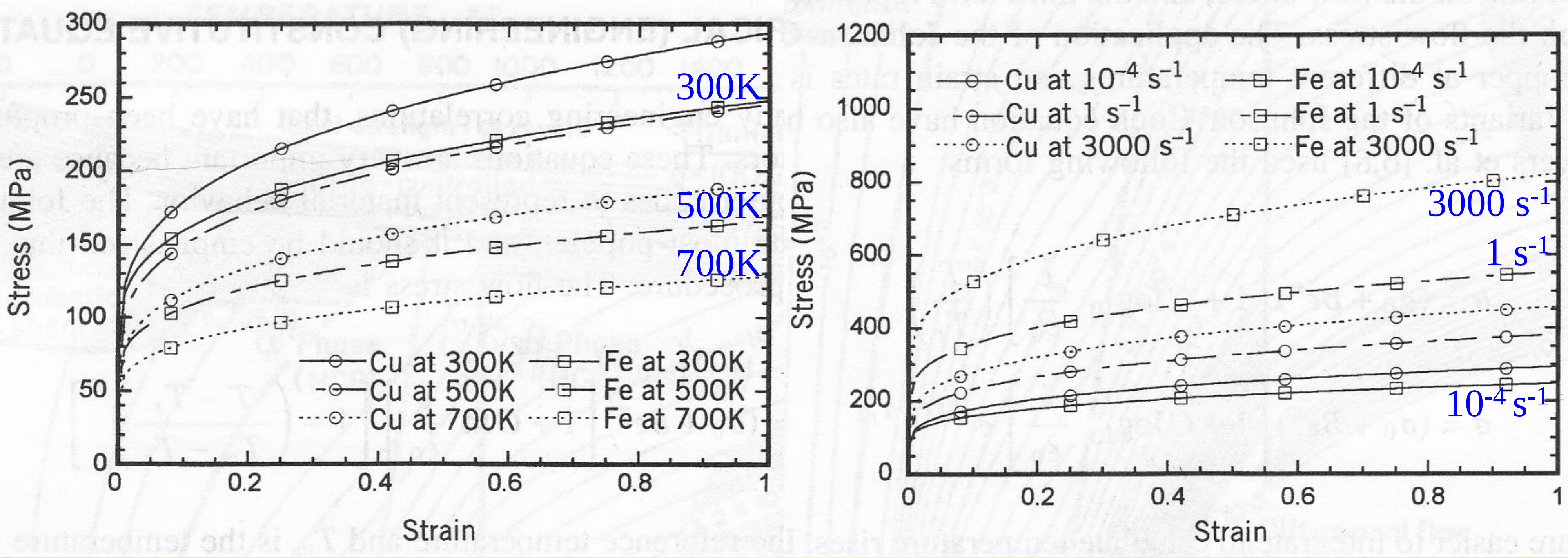
Constitutive Equations: $\sigma = f\left(\varepsilon,\ \frac{d\varepsilon}{dt},\ T,\ deformation\ \ history\right)$

Litonski	1977	$\tau = B(\gamma_0 + \gamma_p)^n (1 - aT)\left[1 + b\left(\frac{d\gamma}{dt}\right)\right]^m$
Johnson-Cook	1983	$\sigma = (\sigma_0 + B\varepsilon^n)\left[1 + C\ln\frac{\dot{\varepsilon}}{\dot{\varepsilon}_0}\right]\left[1 - \left(\frac{T - T_r}{T_m - T_r}\right)^m\right]$
Klopp	1985	$\tau = \tau_0\left(\frac{\gamma}{\gamma_0}\right)^n\left(\frac{T}{T_r}\right)^{-\nu}\left(\frac{\dot{\gamma}_p}{\dot{\gamma}_0}\right)^m => \tau = \tau_0\left(\frac{\dot{\gamma}}{\dot{\gamma}_0}\right)^{1/M}\left(1 + \frac{\gamma}{\gamma_0}\right)^m \exp(-\lambda\Delta T)$
Meyers	1994	$\sigma = (\sigma_0 + B\varepsilon^n)\left[1 + C\log_{10}\frac{\dot{\varepsilon}}{\dot{\varepsilon}_0}\right]\left(\frac{T}{T_r}\right)^{-\lambda}$ $\sigma = (\sigma_0 + B\varepsilon^n)\left[1 + C\log_{10}\frac{\dot{\varepsilon}}{\dot{\varepsilon}_0}\right]e^{-\lambda(T - T_r)}$
Andrade	1994	$\sigma = (\sigma_0 + B\varepsilon^n)\left[1 + C\log\frac{\dot{\varepsilon}}{\dot{\varepsilon}_0}\right]\left[1 - \left(\frac{T - T_r}{T_m - T_r}\right)^m\right]H(T)$ $H(T) = \frac{1}{1 - \{1 - [(\sigma_f)_{rec}/(\sigma_f)_{def}]\}u(T)};\quad u(T) = \begin{cases} 0 & for\ \ T < T_c \\ 1 & for\ \ T > T_c \end{cases}$

M. A. Meyers, in "Mechanics and Materials," John Wiley & Sons, 1999

Experimental Results

- Johnson-Cook Equation to iron $\sigma = \left(\sigma_0 + B\varepsilon^n\right)\left[1 + C\ln\frac{\dot{\varepsilon}}{\dot{\varepsilon}_0}\right]\left[1 - \left(\frac{T - T_r}{T_m - T_r}\right)^m\right]$

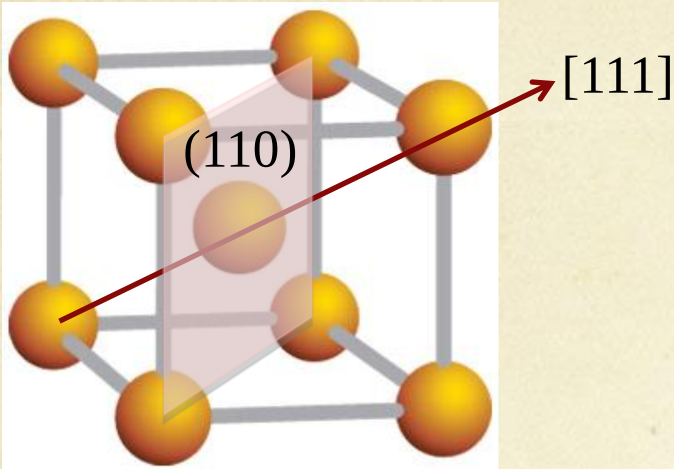


- The rate of work hardening increases for
  - decreasing temperature
  - increasing strain rate

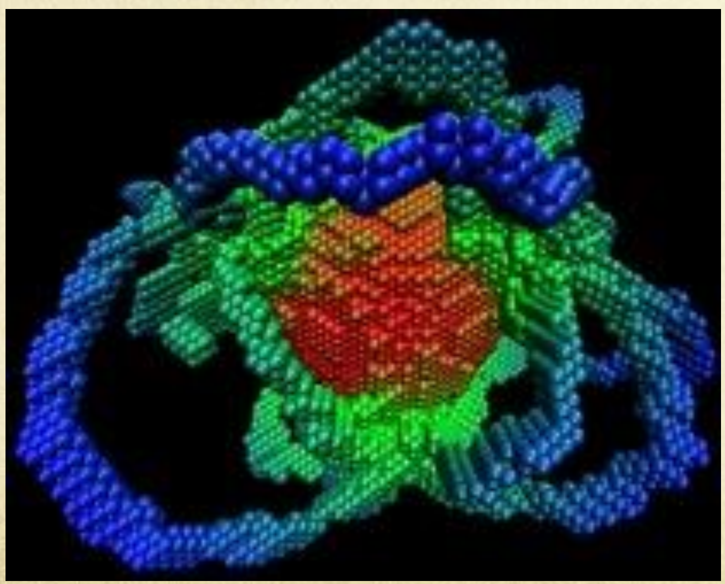
U. R. Andrade, M. A. Meyers, and A. H. Chokshi, Acripta Met. et mat. 30 (1994) 933

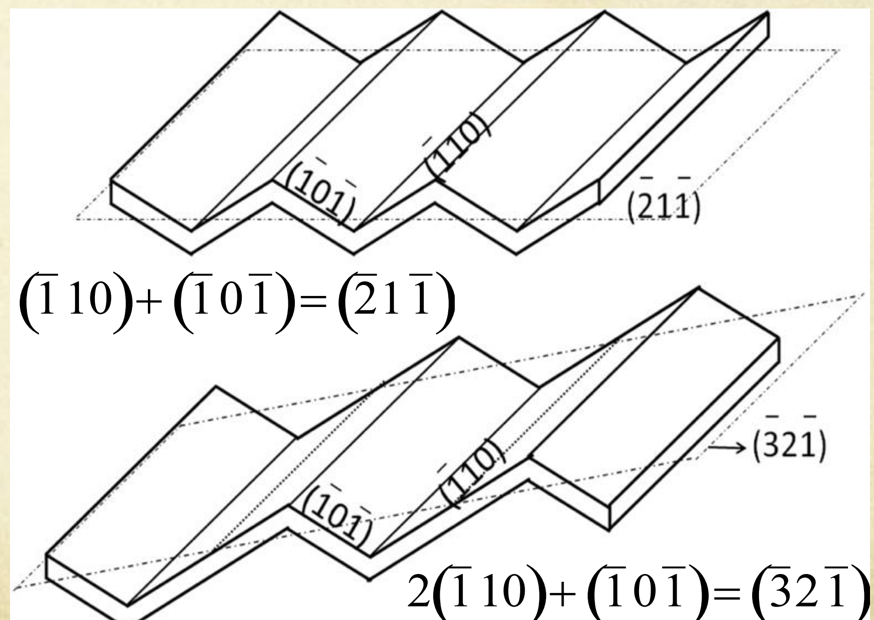
Dynamic Behavior
~ Dislocation Motion ~

BCC Slip Systems



Slip Plane {110}		Slip Plane {112}		Slip Plane {123}			
(110)	$[1\bar{1}1]$	(112)	$[\bar{1}\bar{1}1]$	(123)	$[11\bar{1}]$	(123)	$[\bar{1}11]$
(110)	$[1\bar{1}\bar{1}]$	(121)	$[1\bar{1}1]$	(132)	$[1\bar{1}1]$	(132)	$[\bar{1}11]$
$(1\bar{1}0)$	$[11\bar{1}]$	(211)	$[\bar{1}11]$	(312)	$[\bar{1}11]$	(312)	$[1\bar{1}1]$
(110)	[111]	$(11\bar{2})$	[111]	(321)	$[\bar{1}11]$	(321)	$[11\bar{1}]$
$(10\bar{1})$	[111]	$(1\bar{2}1)$	[111]	(213)	$[11\bar{1}]$	(213)	$[1\bar{1}1]$
$(10\bar{1})$	$[1\bar{1}1]$	$(\bar{2}11)$	[111]	(231)	$[1\bar{1}1]$	(231)	$[11\bar{1}]$
(101)	$[11\bar{1}]$	$(1\bar{1}2)$	$[1\bar{1}\bar{1}]$	(123)	[111]	$(\bar{1}23)$	$[1\bar{1}1]$
(101)	$[1\bar{1}\bar{1}]$	$(12\bar{1})$	$[1\bar{1}\bar{1}]$	(132)	[111]	$(\bar{1}32)$	$[11\bar{1}]$
(011)	$[11\bar{1}]$	$(21\bar{1})$	$[\bar{1}1\bar{1}]$	(312)	[111]	$(3\bar{1}2)$	$[11\bar{1}]$
(011)	$[\bar{1}11]$	$(\bar{1}12)$	$[\bar{1}1\bar{1}]$	(312)	[111]	$(32\bar{1})$	$[1\bar{1}1]$
$(0\bar{1}1)$	[111]	$(\bar{1}21)$	$[11\bar{1}]$	(213)	[111]	$(2\bar{1}3)$	$[\bar{1}11]$
$(0\bar{1}1)$	$[\bar{1}11]$	$(2\bar{1}1)$	$[11\bar{1}]$	(231)	[111]	$(23\bar{1})$	$[\bar{1}11]$

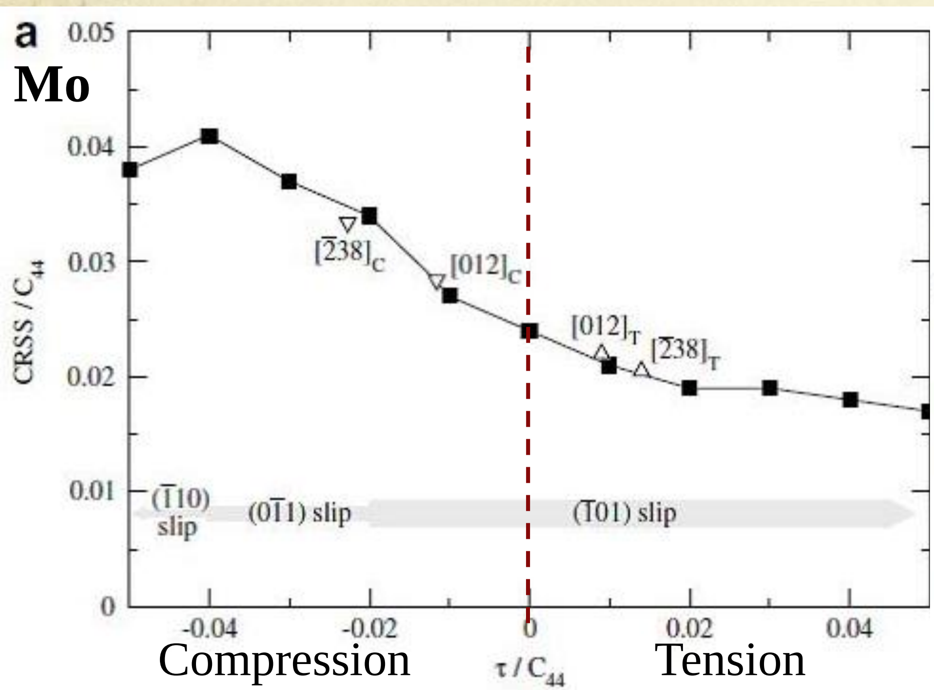


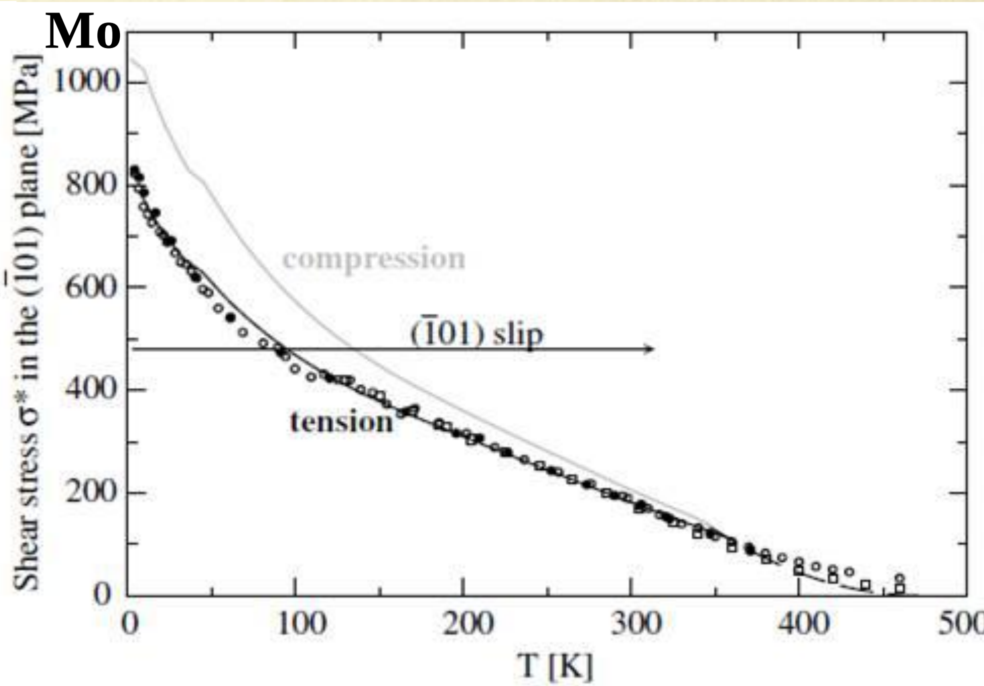


Y. Tang, E. M. Bringa, B. A. Remington, M. A. Meyers, Acta Mat. (2010). Imprint
M. A. Meyers and K. K. Chawla, in "Mechanics Behavior of Materials," Prentice-Hall, 1999

Asymmetry in Dislocation Glide

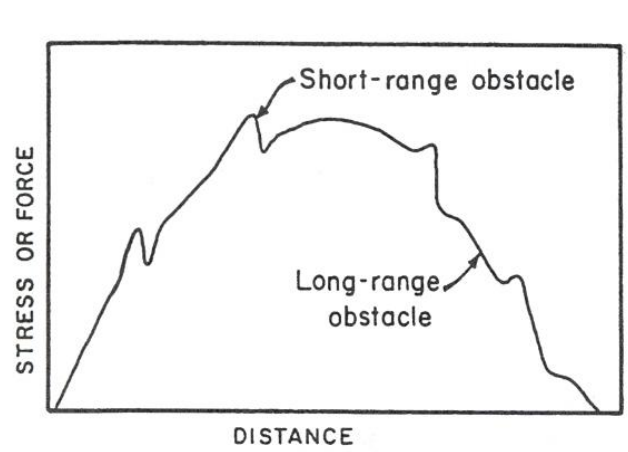
- Core dislocation structure: ½[111] screw dislocation
- Maximum resolved shear stress plane (MRSSP) is $(\bar{1}01)$

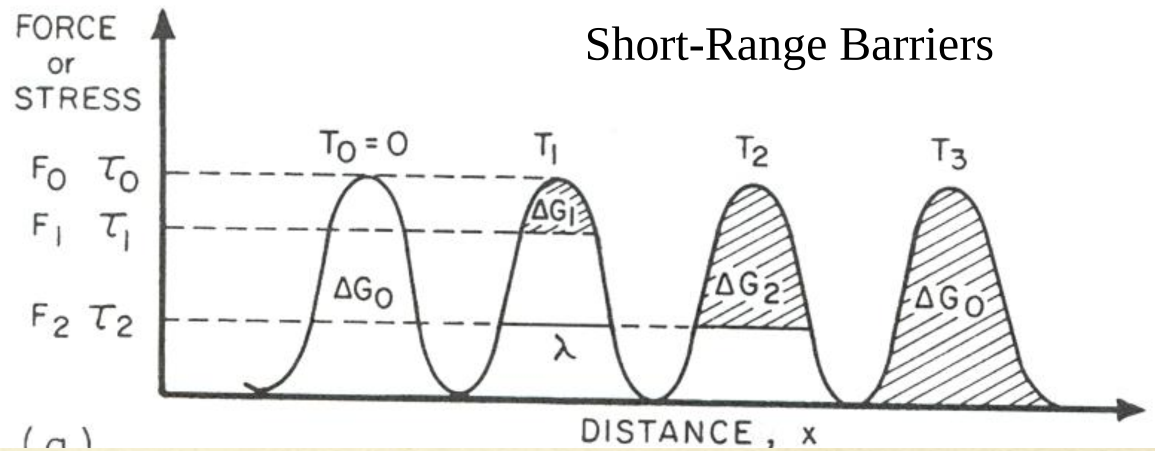




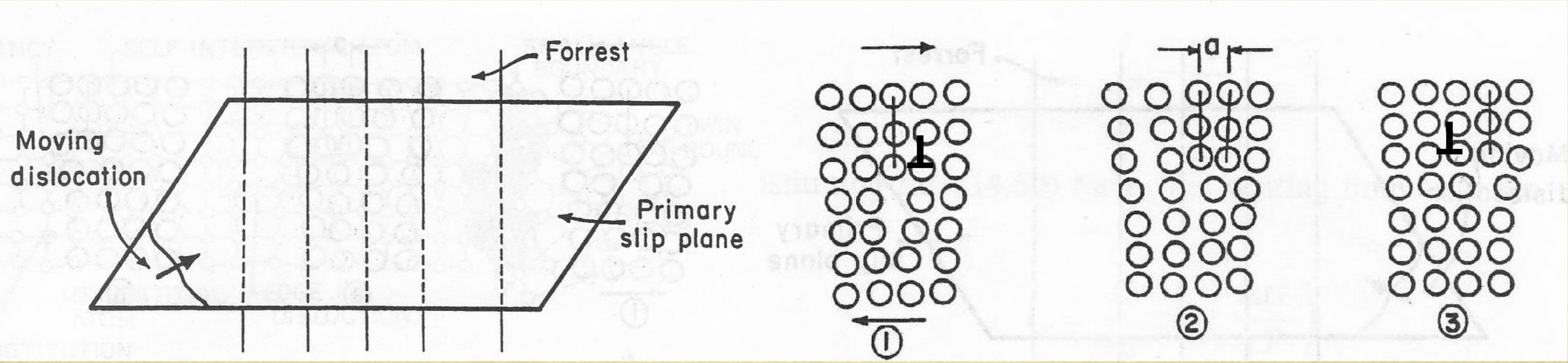
R. Groger, A. G. Bailey, V. Vitek, Acta Mater. 56 (2008) 5401
R. Groger, A. G. Bailey, V. Vitek, Acta Mater. 56 (2008) 5426
Vitek and Paidar, in "Dislocation in Solids", Vol. 14, Ch. 87, 2008

Barriers to Dislocation Motion





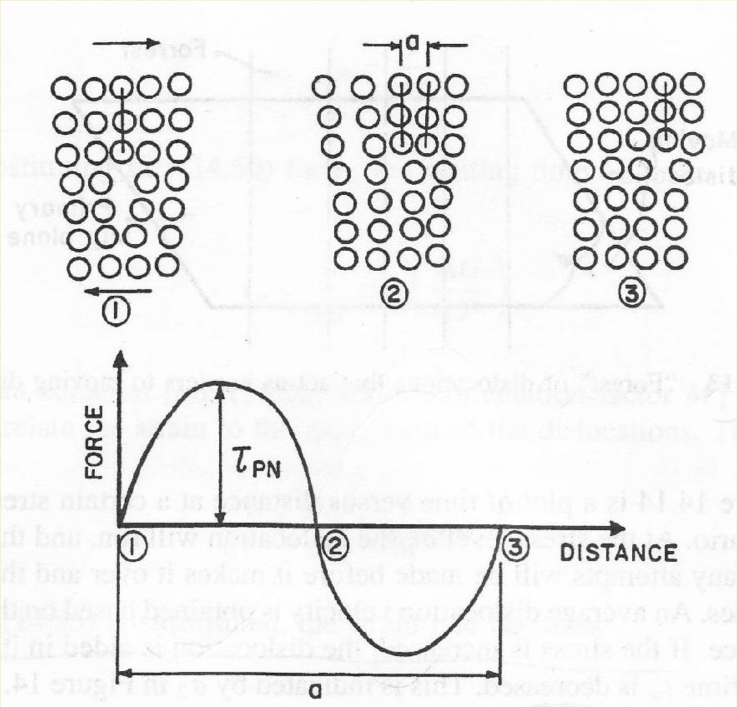
Rate Controlling Mechanisms	
FCC	BCC
Dislocation Forests	Peierls-Nabarro Barrier
$\upsilon^* \sim 100-1000b^3$	$\upsilon^* \sim 10-100b^3$



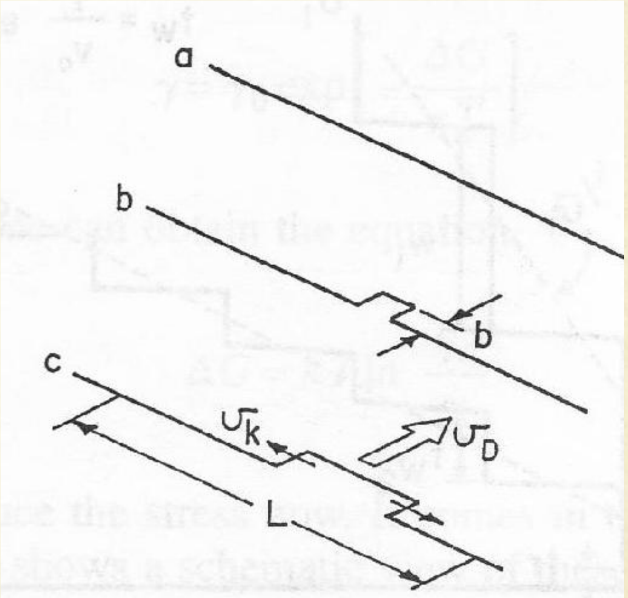
C. Duhamel, Y. Brechet, and Y. Champion, Inter. J. Plasticity 26 (2010) 747
P. S. Follansbee, Metall. Mater. Tans. A, 41A (2010) 3080
B. Xu, Z. Yue, and X. Chen, J. Phys. D: Appl/ Phys. 43 (2010) 245401

Dislocation Movement

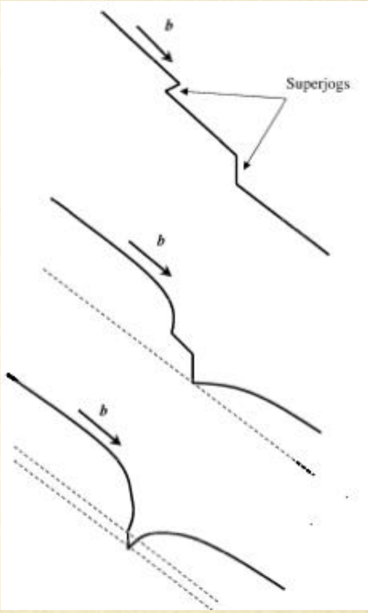
- Peierls-Nabarro barrier



- Seeger kink-pair Mechanism



- Pinning

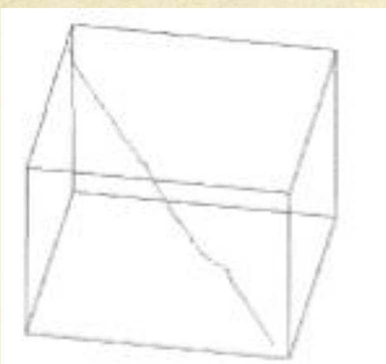


M. Rhee, D. Lassila, V. V. Bulatov, L. Hsiung, and T. D. Rubia, Philo. Mag. Lett. Vol. 81 (2001) 595

Dislocation Movement

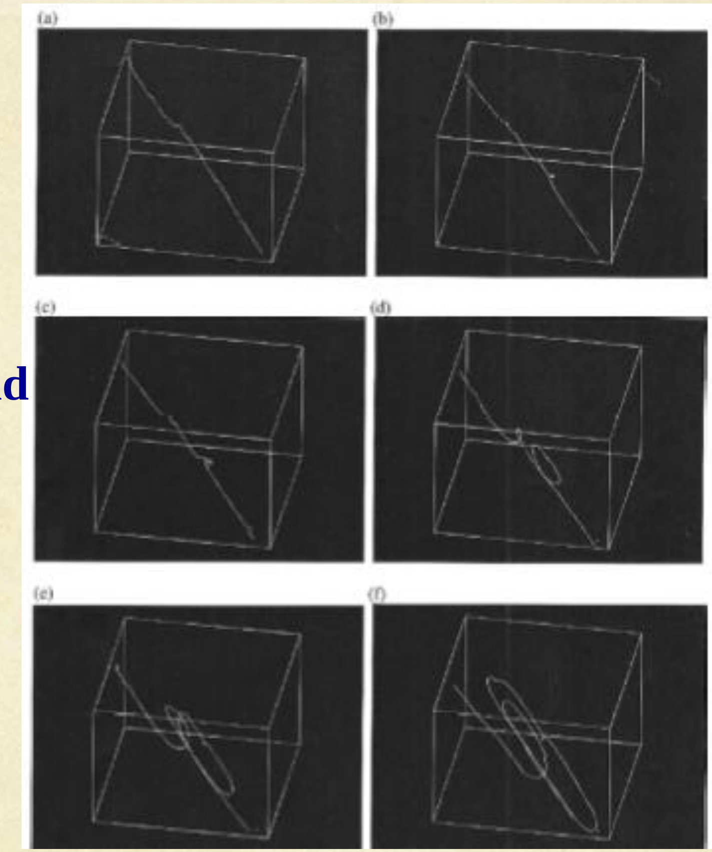
BCC Molybdenum (Mo)

Uniaxial stress applied along the [001] axis

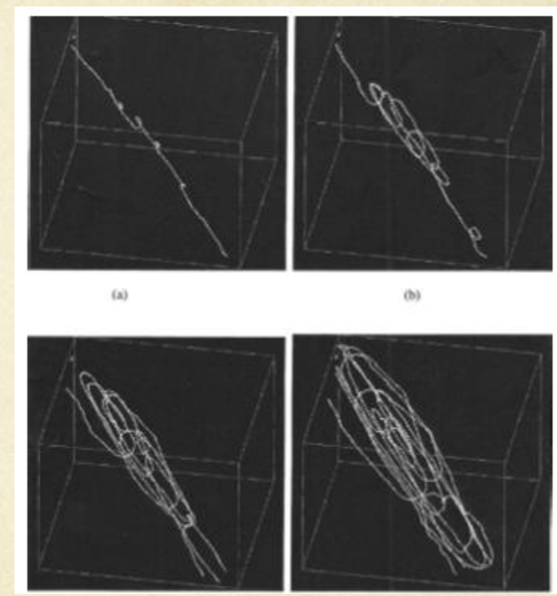


50 MPa

threshold stress



200 MPa

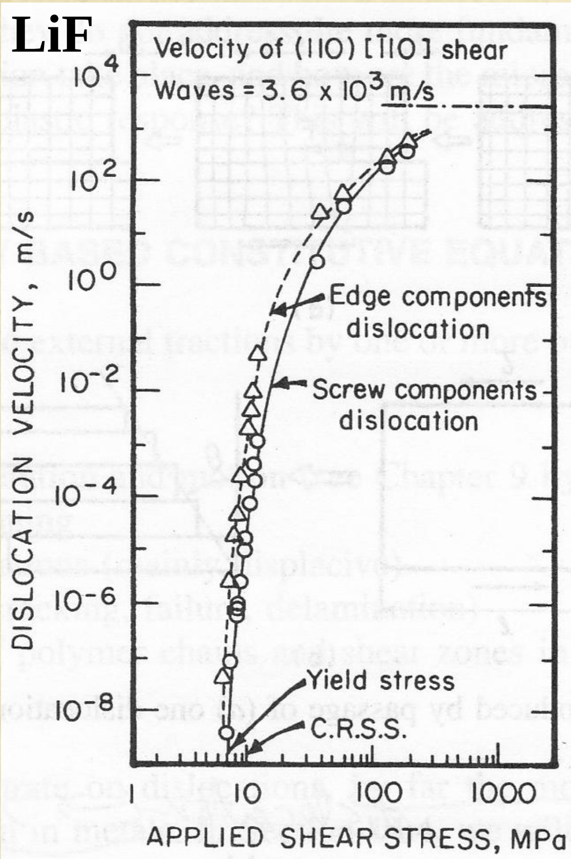


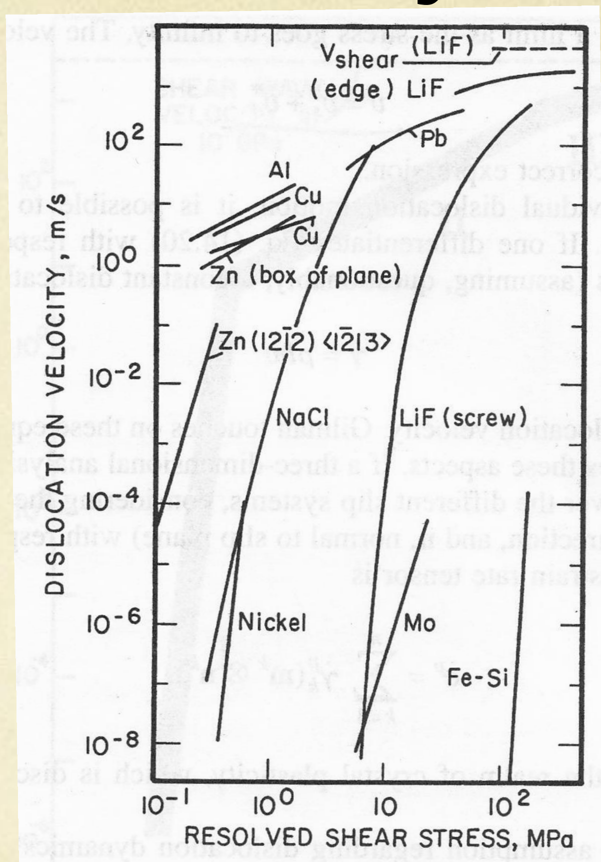
1000 MPa

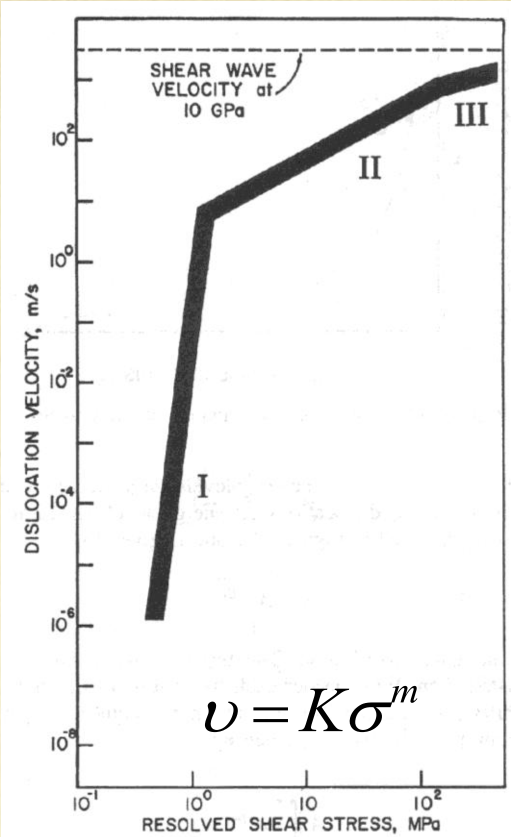
Stress (MPa)

M. Rhee, D. Lassila, V. V. Bulatov, L. Hsiung, and T. D. Rubia, Philo. Mag. Lett. Vol. 81 (2001) 595

Dislocation Dynamics







$$\upsilon = K\sigma^m$$

Johnston and Gilman	1959	$\upsilon \propto \tau^m e^{-Q/kT}$
Stein and Low	1960	$\upsilon = \upsilon_0 \exp\left(-\frac{A}{\tau}\right)$
Rohde and Pitt	1967	$\upsilon = \frac{kT}{h} K \exp\left(-\frac{\Delta H}{kT}\right)\exp\left[\frac{B(\tau_a - \tau_\ell)}{kT}\right]$ for iron
Gilman	1968	$\upsilon = \upsilon_s^*\left(1 - e^{-\tau/s}\right) + \upsilon_d^* e^{-D/\tau}$

Region I: Thermal activation

$m_I > 1$

Region II: Drag (Viscous glide)

$m_{II} = 1$

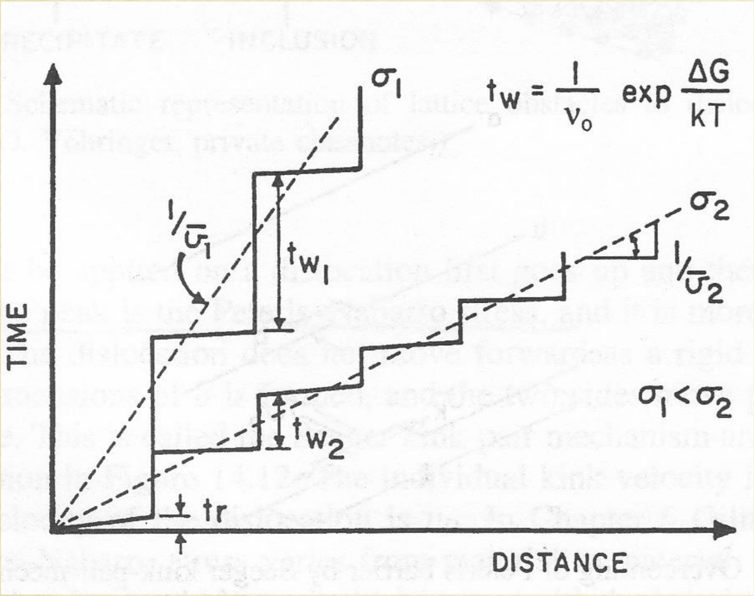
Region III: Relativistic effects

$m_{III} < 1$

W. G. Johnston and J. J. Gilman, J. Appl. Phys. 33 (1959) 132

Dislocation Behavior – Region I

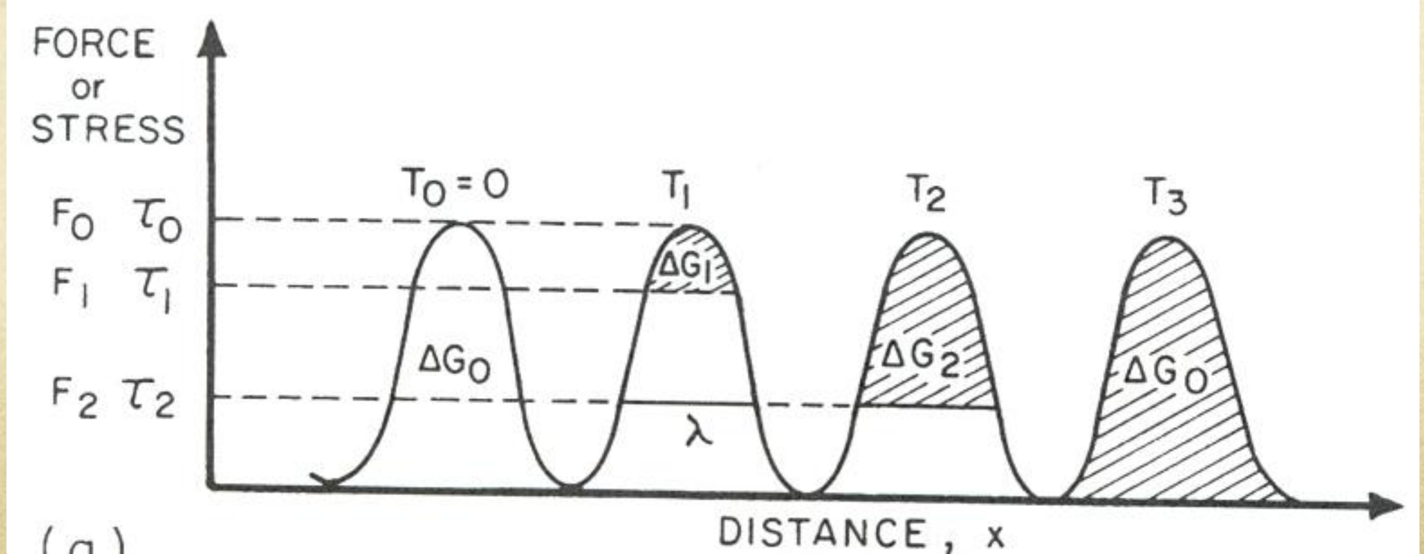
- Physical based constitutive equation



- Apply Orowan equation: $\dot{\gamma} = \dot{\gamma}_0 \exp\left[-\frac{\Delta G}{kT}\right]$
- At T_1: $\Delta G = \Delta G_0 - \Delta G_1$

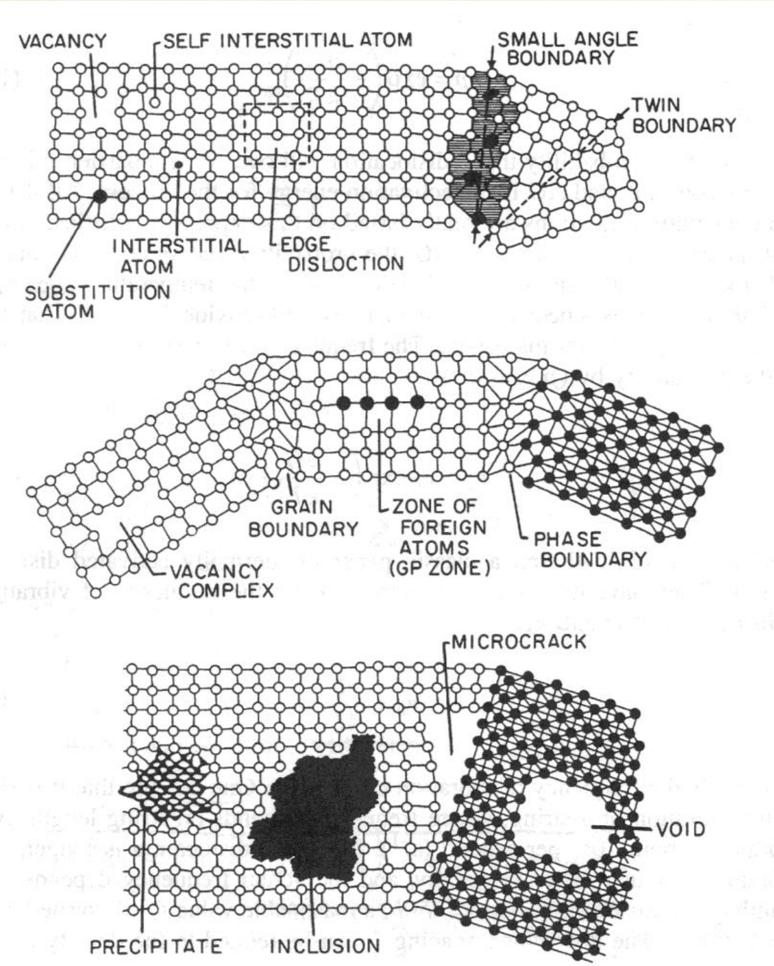
$$kT \ln \frac{\dot{\gamma}_0}{\dot{\gamma}} = \Delta G_0 - \int_{F_i}^{F_0} \lambda(F)\, dF$$

$$\tau = \tau_G + \frac{\Delta G_0}{V} + \frac{kT}{V} \ln \frac{\dot{\gamma}}{\dot{\gamma}_0}$$



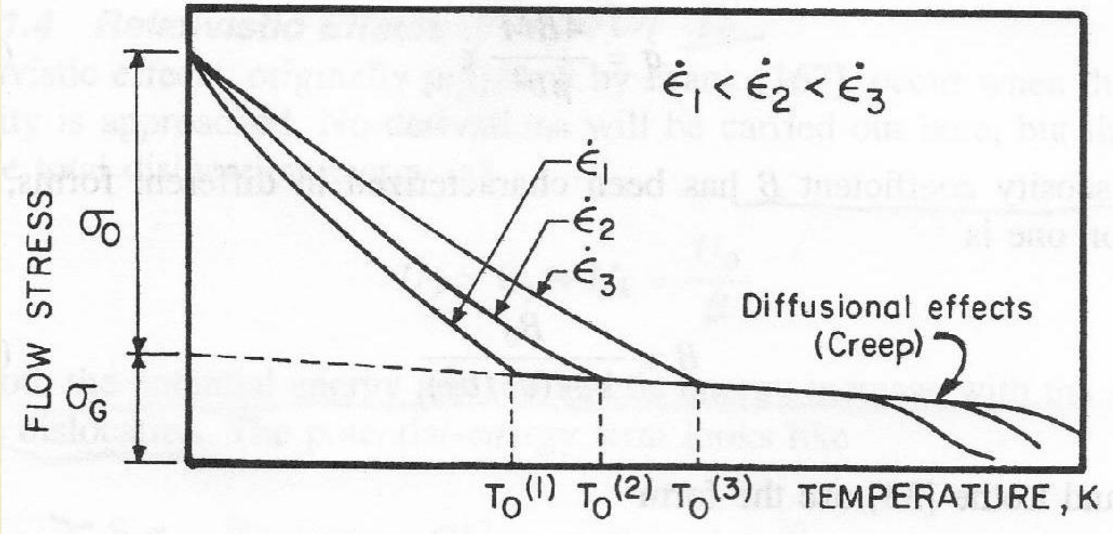
- For different barrier shape, Kocks et al. proposed a generalized equation $\Delta G = \Delta G_0 \left[1 - \left(\frac{\sigma}{\sigma_0} \right)^p \right]^q$

➔ MTS Model (LANL): $\left(\frac{\sigma}{G(T)} \right)^P = \left(\frac{\sigma_0}{G(T)} \right)^P \left[1 - \left(\frac{kT}{Gb^3 g_0} \ln \frac{\dot{\varepsilon}}{\dot{\varepsilon}_0} \right)^{1/q} \right]$



- Generalized Constitutive Equation

$$kT \ln \frac{\dot{\varepsilon}_0}{\dot{\varepsilon}} = \Delta G_0 \left[1 - \left(\frac{\sigma}{\sigma_0} \right)^p \right]^q$$



- Athermal: very small temperature dependence

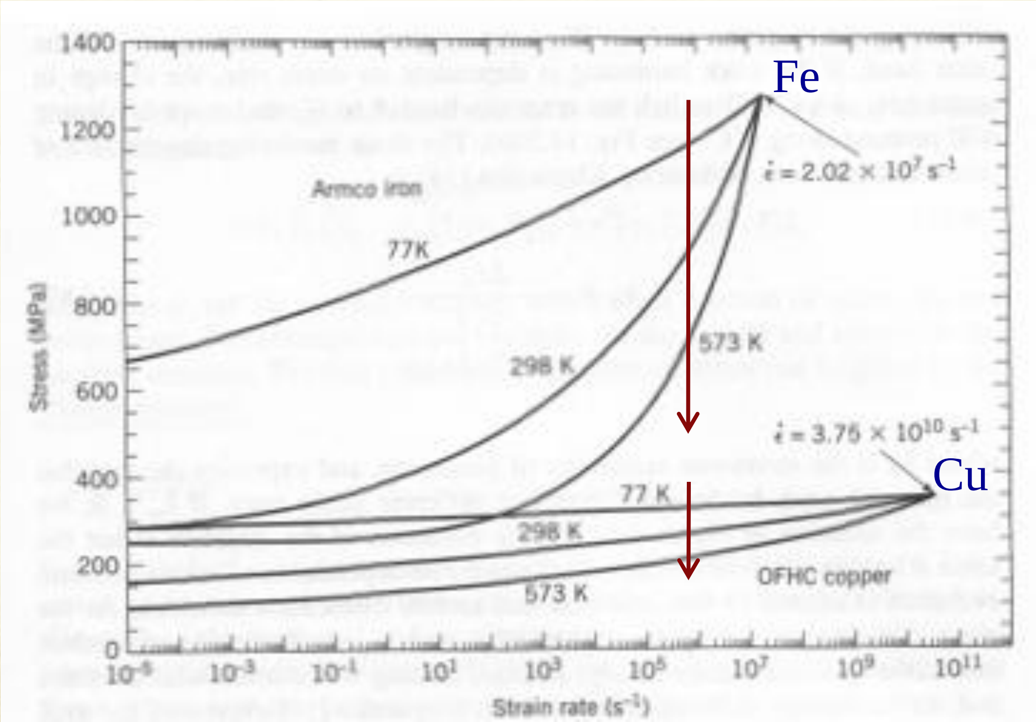
Schematic representation of lattice obstacles to dislocation motion adapted from O. Vohringer, private classnotes
M. A. Meyers, in "Mechanics and Materials," John Wiley & Sons, 1999

Zerilli-Armstrong Equation

- Two microstructurally based constitutive equations:

  Activation area constant in BCC: $\sigma^* = C_1 \exp\left(-C_3 T + C_4 T \ln \dot{\varepsilon}\right)$
- Hall-Petch equation: (D is the grain size) $\sigma = \sigma_G + \sigma^* + kD^{-1/2}$
- Zerilli-Armstrong equation for BCC metals:

$$\sigma = \sigma_G + \sigma^* + kD^{-1/2} = \sigma_G + C_1 \exp\left(-C_3 T + C_4 T \ln \dot{\varepsilon}\right) + C_5 \varepsilon^n + kD^{-1/2}$$



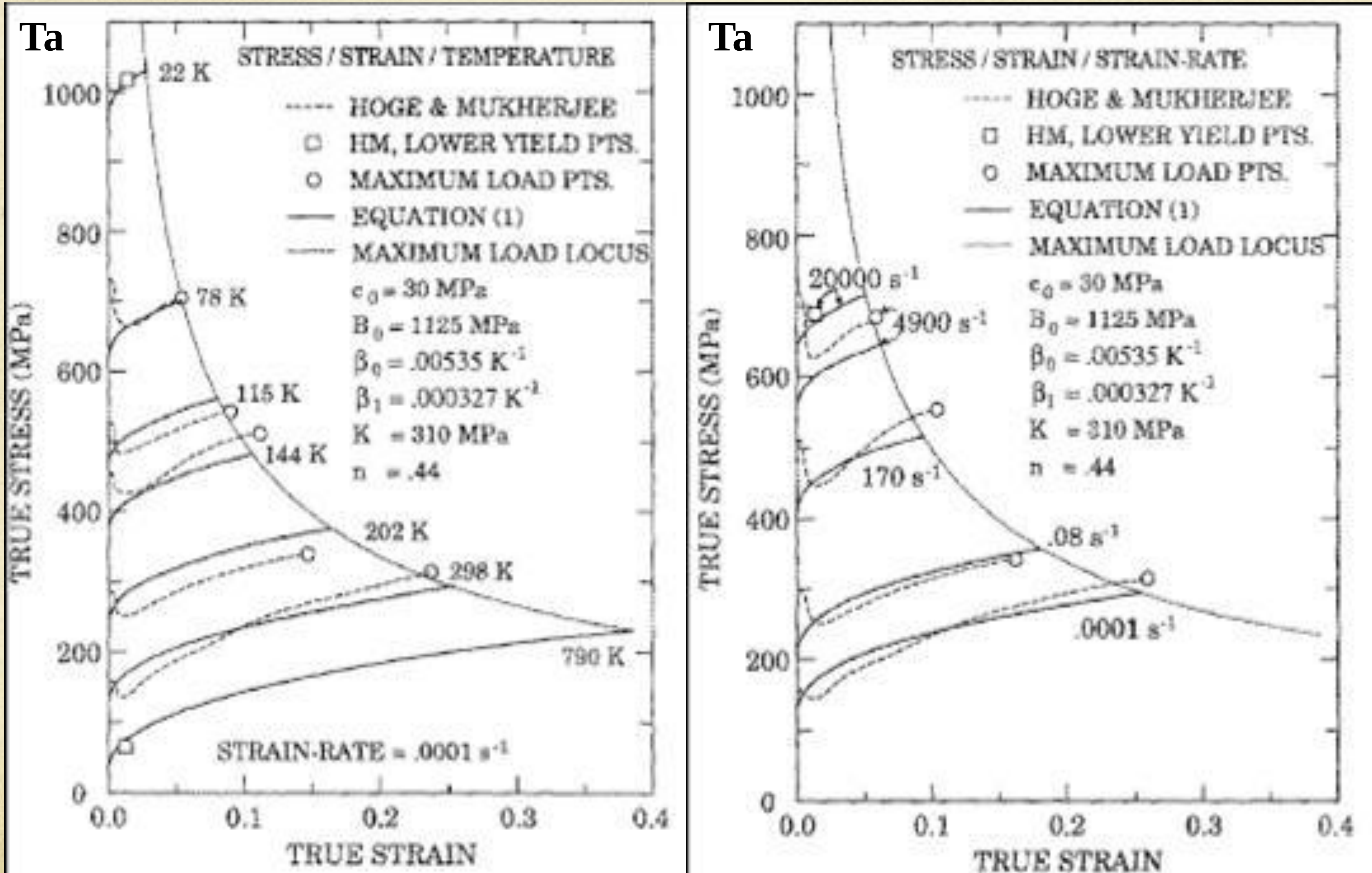
F. J. Zerilli and R. W. Armstrong, J. Appl. Phys. 68(4), 1990

M. A. Meyers, in "Mechanics and Materials," John Wiley & Sons, 1999

Maximum load (true) strain as a function of strain rate and temperature

$$\sigma = \sigma_G + \sigma^* + kD^{-1/2} = \sigma_G + C_1 \exp\left(-C_3 T + C_4 T \ln \dot{\varepsilon}\right) + C_5 \varepsilon^n + kD^{-1/2}$$

$$C_5\left(\varepsilon^n - n\varepsilon^{n-1}\right) + \sigma_G + C_1 \exp\left(-C_3 T + C_4 T \ln \dot{\varepsilon}\right) + kD^{-1/2} = 0$$



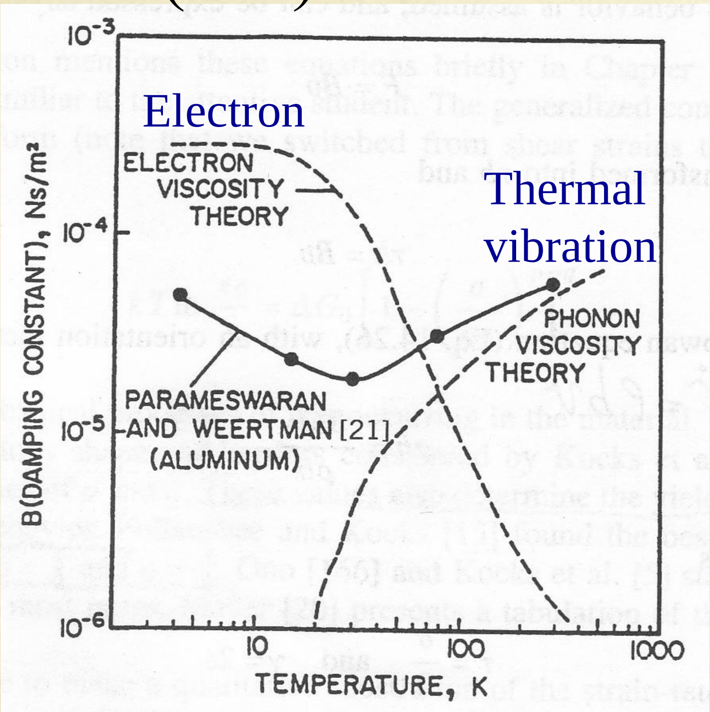
F. J. Zerilli and R. W. Armstrong, J. Appl. Phys. 68(4), 1990

Dislocation Behavior – Region II

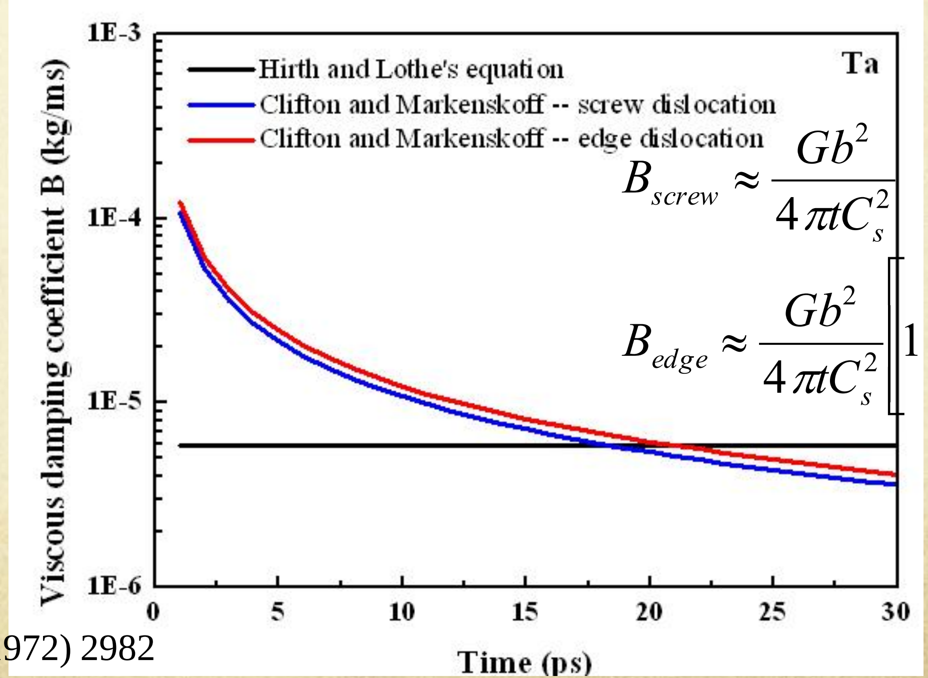
- Drag Regime
  - Newtonian viscous behavior is assumed $f_v = Bv$

    and using Orowan equation with orientation factor, $\sigma = \frac{4BM}{\rho b^2}\dot{\varepsilon}$
  - Hirth and Lothe: viscosity coefficient from phonon viscosity

$$B = \frac{B_0}{1-\left(\upsilon^2/\upsilon_S^2\right)} \approx \frac{bw}{10\upsilon_e} = \frac{b}{10\upsilon_e}\frac{3kT}{a^3}$$



- Clifton and Markenskoff: additional damping mechanisms due to the inertial resistance of a dislocation to motion



$$B_{screw} \approx \frac{Gb^2}{4\pi t C_s^2}$$

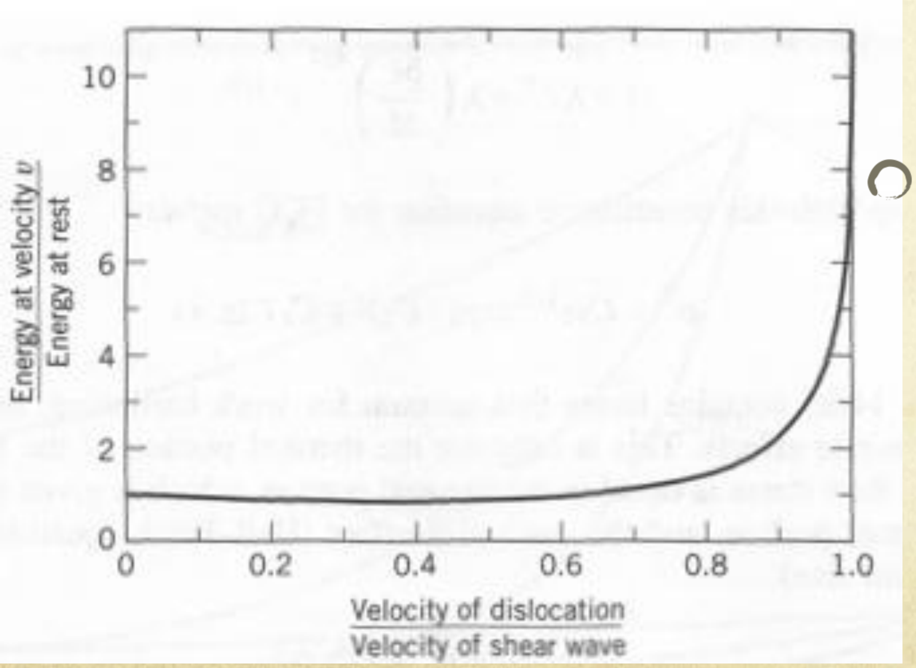
$$B_{edge} \approx \frac{Gb^2}{4\pi t C_s^2}\left[1+\left(\frac{C_s}{C_l}\right)^4\right]$$

Parameswaran, N. Urabe, and J. Weertman, JAP 43 (1972) 2982

R. J. Clifton and X. Markenscoff, J. Mech. Phys. Solids, 29 (1981) 227

Dislocation Behavior – Region III

- Relativistic Effects
  - Occur when the sound velocity is approached
  - Frank: total dislocation energy $U_T = U_P + U_k = \frac{U_0}{\beta}$
  - Weertman: potential-energy $U_P = \frac{Gb^2}{4\pi} \ln\left(\frac{R}{r_0}\right) \frac{1+\beta^2}{2\beta}$ where $\beta = \left(1 - \frac{\upsilon^2}{\upsilon_s^2}\right)^{1/2}$



- Dislocation velocity approached shear wave velocity, energy of the dislocation goes to infinity.

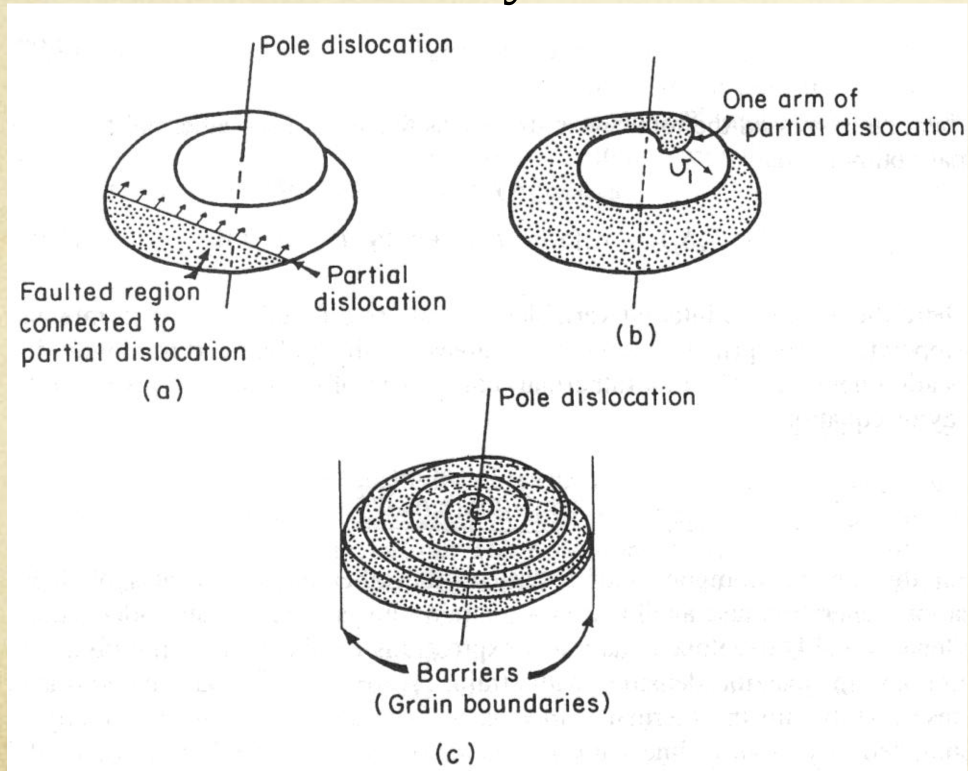
M. A. Meyers, in "Mechanics and Materials," John Wiley & Sons, 1999

Dynamic Behavior
~ Mechanical Twinning ~

Twinning Mechanisms

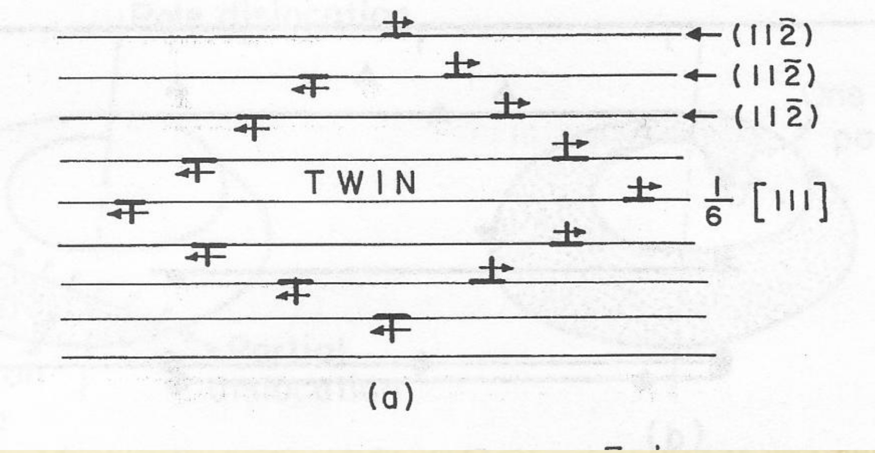
- Mechanical twinning and slip are competing mechanisms
- Favored at low temperatures and high strain rates
- Twin mechanisms for BCC metals:

- Cottrell and Bilby: Pole mechanism



A. H. Cottrell and B. A. Bilby, Phil. Mag. 42 (1951), 573

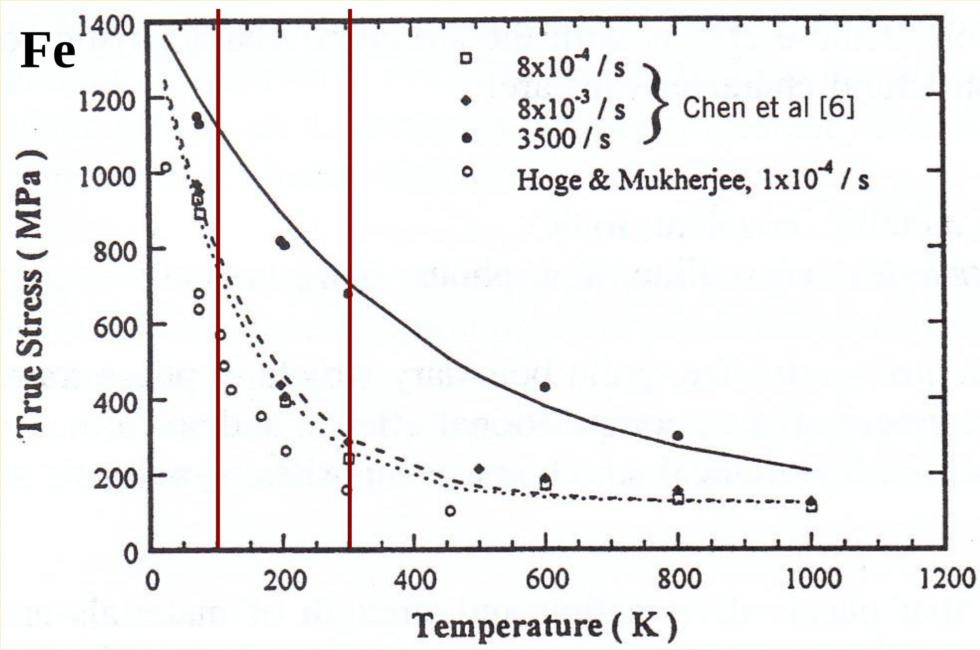
- Sleeswyk:

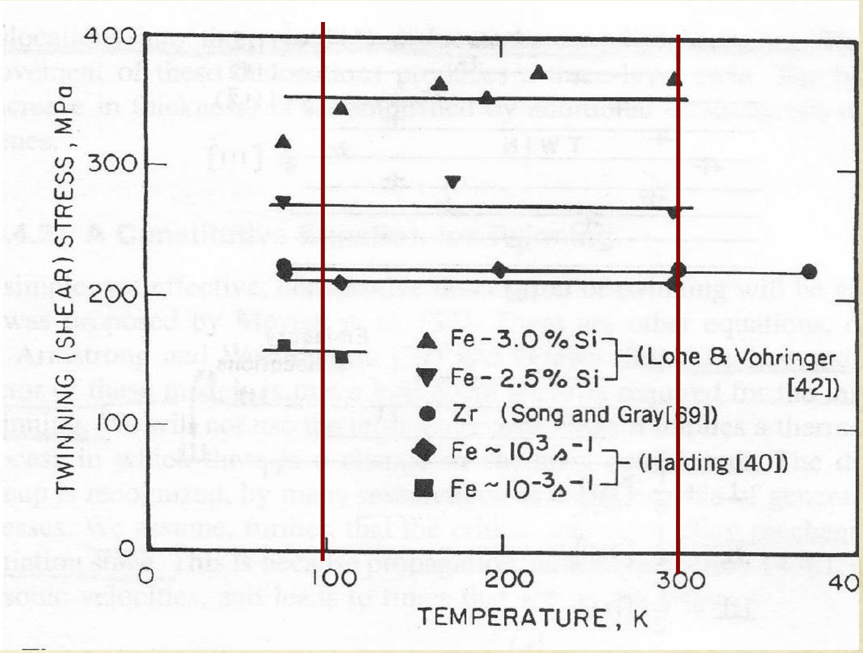


A. W. Sleeswyk, Acta Met. 10 (1962), 803

Mild Temperature Effect

- Dislocation Motion
- Twin Motion



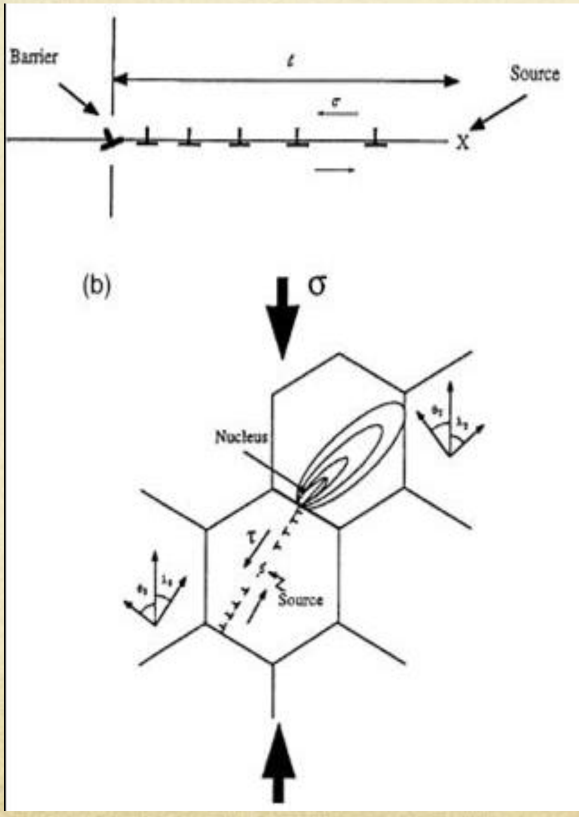


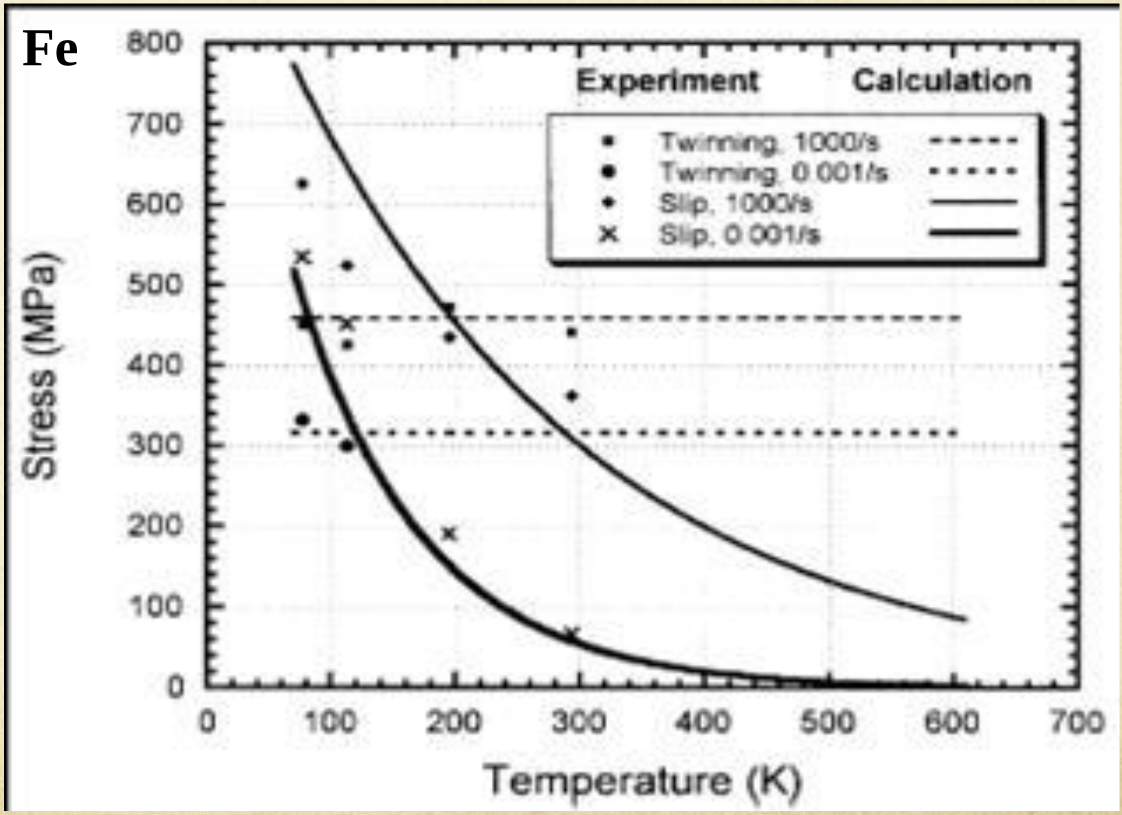
M. A. Meyers, O. Vohringer and V. A. Lubarda, Acta Mater. 49 (2001) 4025
M. A. Meyers, Y. -J. Chen, F. D. S. Marquis, and D. S. Kim, Met. Trans. 26A, (1995) 2493

Constitutive Equation for Twinning

- Consider dislocation pileup: (a high local stress is required)
  - Frank-Read or a Koehler source
    - Individual dislocation (Johnston and Gilman): $\upsilon = A\tau^m e^{-Q/kT}$

$$\sigma_T = 2\left(\frac{n^* LE}{2A}\right)^{1/(m+1)} \dot{\varepsilon}^{1/(m+1)} e^{Q/(m+1)RT} = K'\dot{\varepsilon}^{1/(m+1)} e^{Q/(m+1)RT}$$





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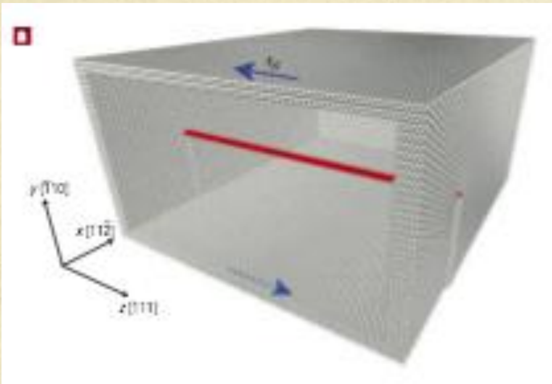
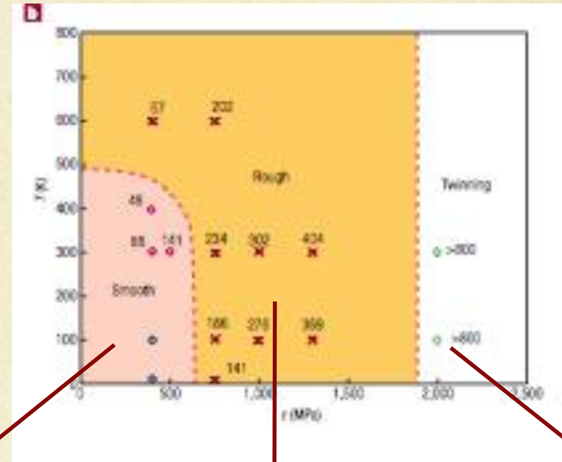
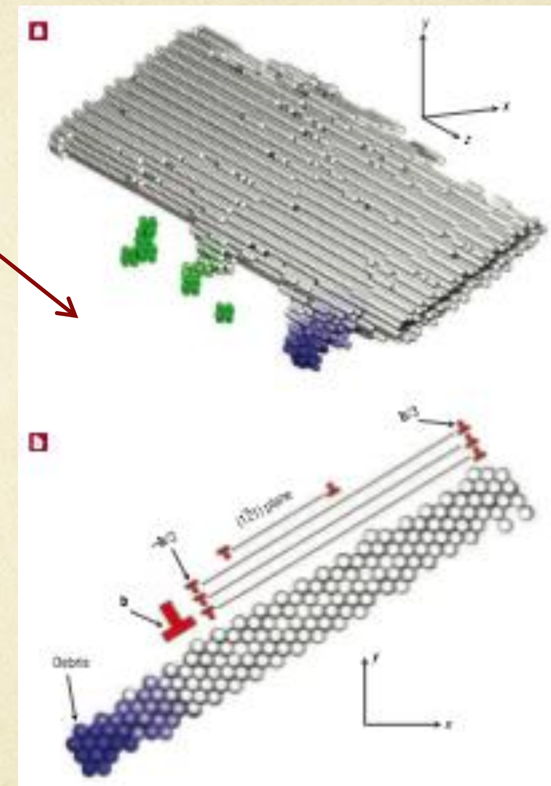
M. A. Meyers, O. Vohringer, and Y. G. Chen, in "Advances in Twinning," TMS-AIME, 1999, p.43

Slip-Twinning Transition (MD)

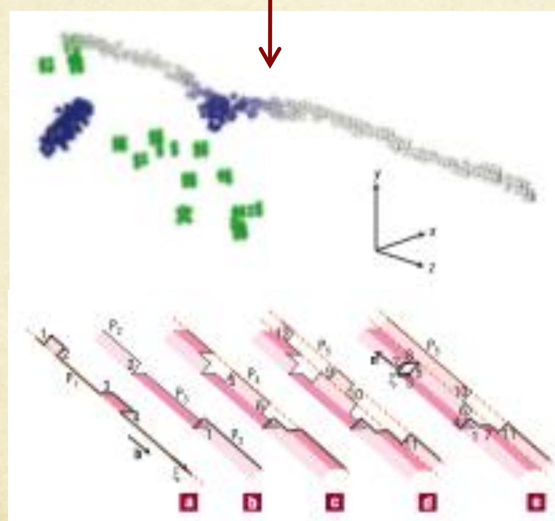
- Screw dislocation in BCC iron (Fe)







- Atomic-sized kink



- Pinning points
- Twinning

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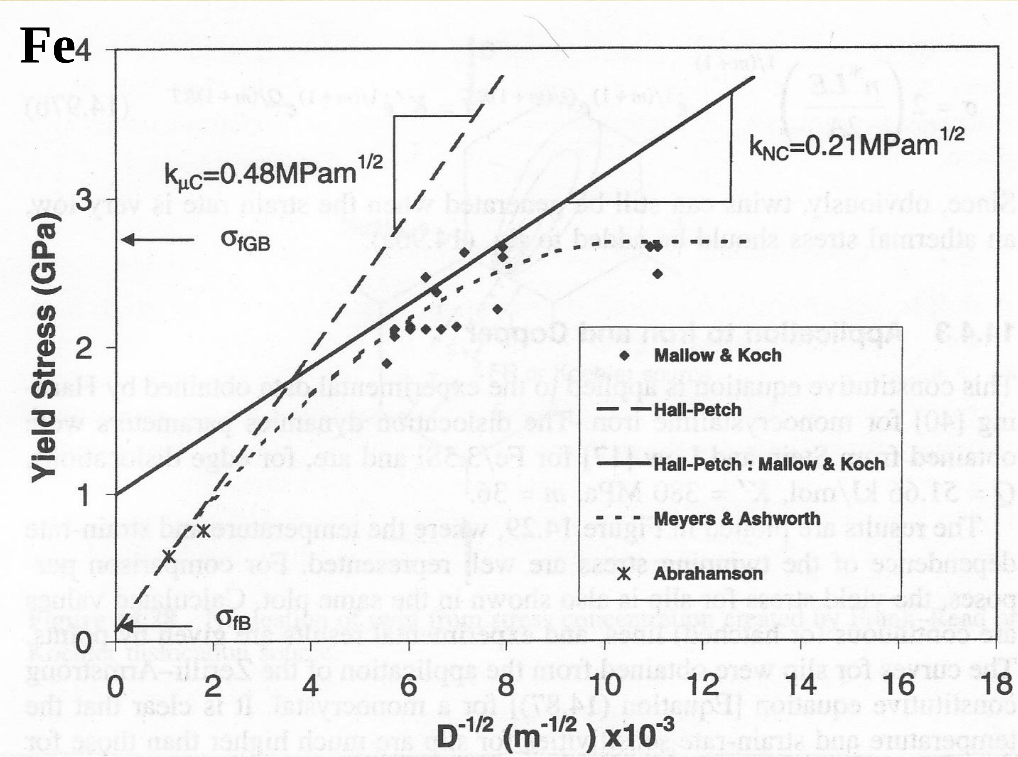
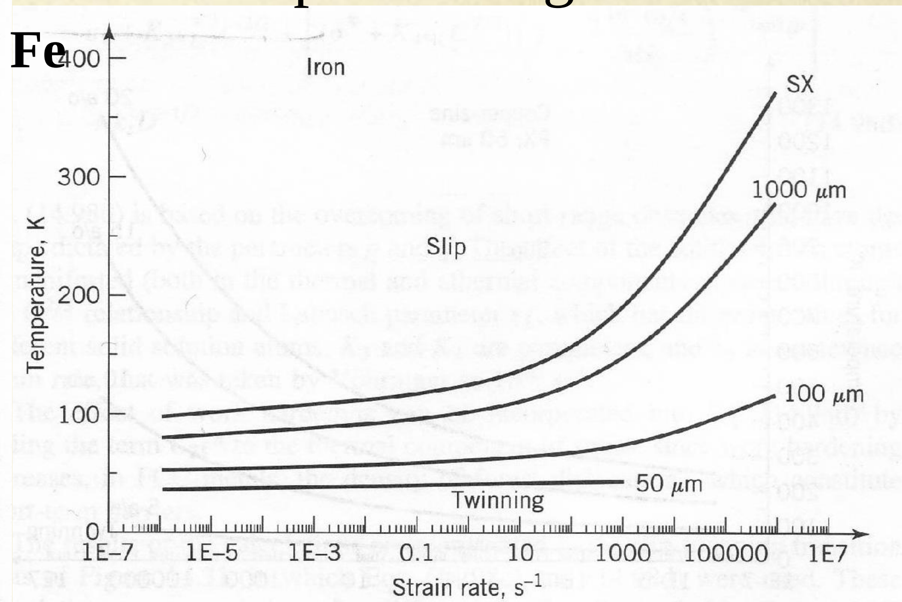
Dynamic Behavior
~ Grain Size Effects ~

Grain Size Effect

- Hall-Petch-like Relationship: $\sigma_T = \sigma_{0T} + k_T d^{-1/2}$
- Meyers-Ashworth Equation: $\sigma_y = \sigma_{fB} + 8k(\sigma_{fGB} - \sigma_{fB})D^{-1/2} - 16k^2(\sigma_{fGB} - \sigma_{fB})D^{-1}$



- The effect of grain size on the slip-twinning transition



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E. P. Abrahamson, II, in Surfaces and Interfaces, Syracuse U. Press, 1968, p. 262
F. J. Zerilli and R. W. Armstrong, J. Appl. Phys. 68(4), 1990
M. A. Meyers, in “Mechanics and Materials,” John Wiley & Sons, 1999

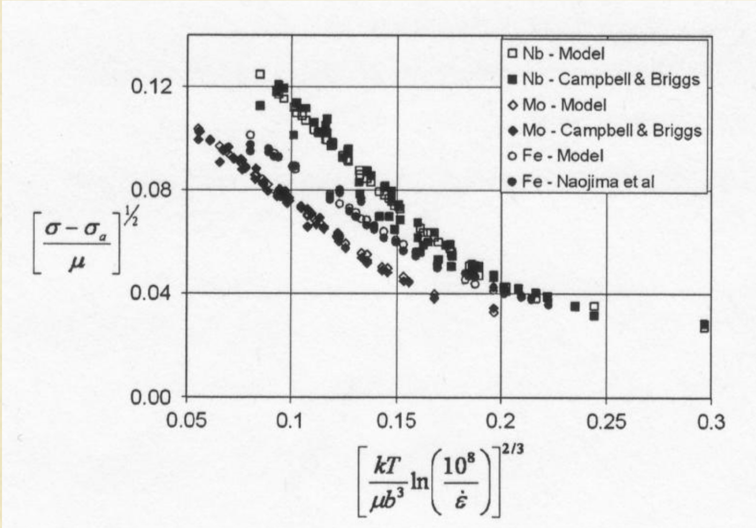
Dynamic Behavior
~ Impurity Effects ~

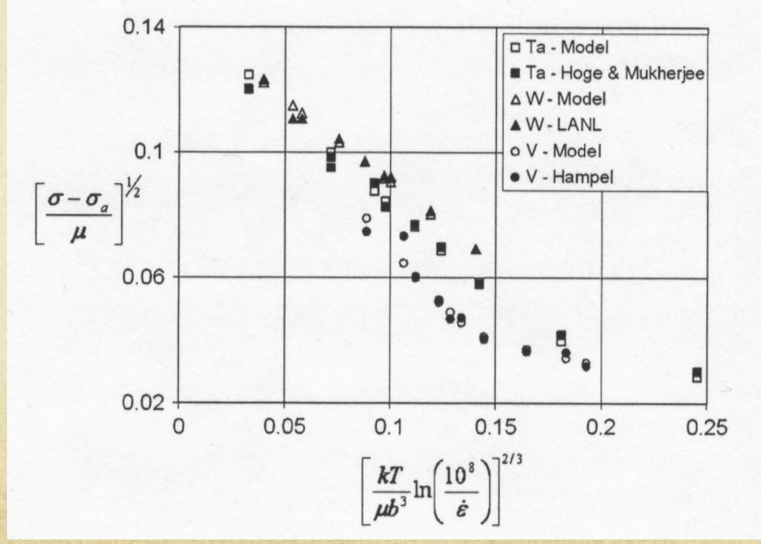
Two-Obstacle Model

- $\sigma = \sigma_a + \sigma_p + \sigma_i$: $\dfrac{\sigma}{\mu} = \dfrac{\sigma_a}{\mu} + S_p(\dot{\varepsilon},T)\dfrac{\hat{\sigma}_p}{\mu_0} + S_i(\dot{\varepsilon},T)\dfrac{\hat{\sigma}_i}{\mu_0}$

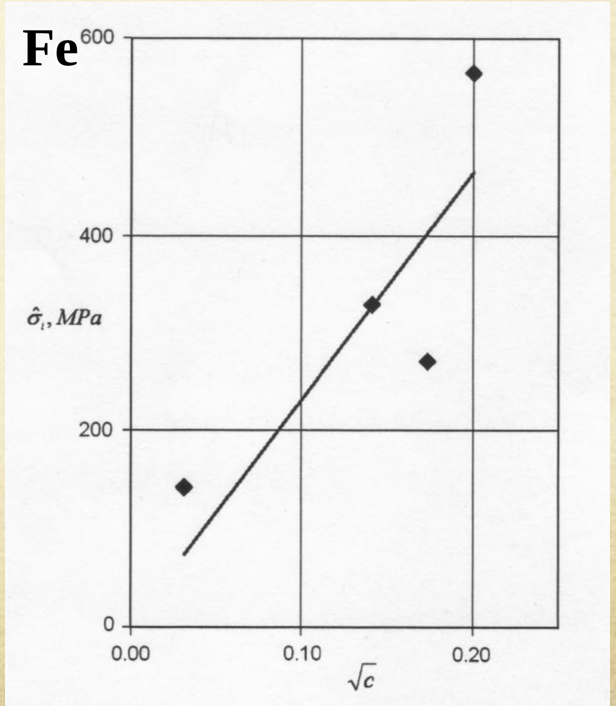
$$\text{where} \quad S_{p,i}(\dot{\varepsilon},T) = \left\{1 - \left[\frac{kT}{\mu b^3 g_{0p,i}} \ln\left(\frac{\dot{\varepsilon}_{0p,i}}{\dot{\varepsilon}}\right)\right]^{1/q}\right\}^{1/p}$$

$$Varshni: \quad \mu(T) = \mu_0 - s/\left(\exp\left(\frac{T_t}{T}\right) - 1\right)$$





- Strength of the obstacle vs. square root of the carbon concentration

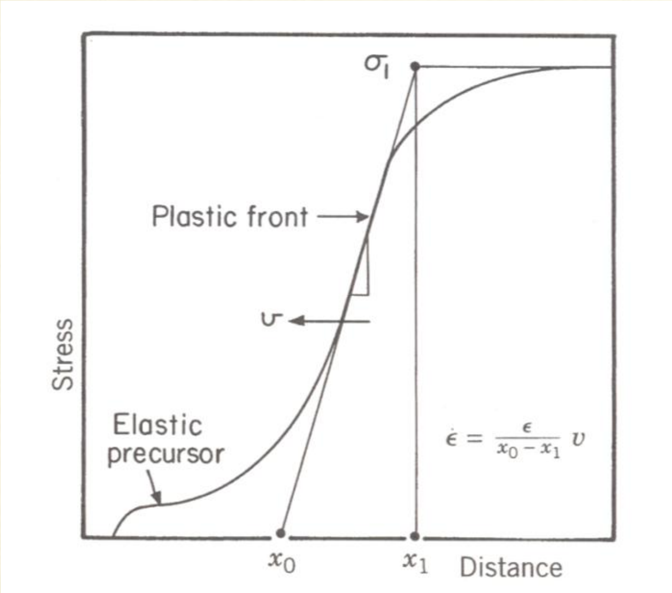


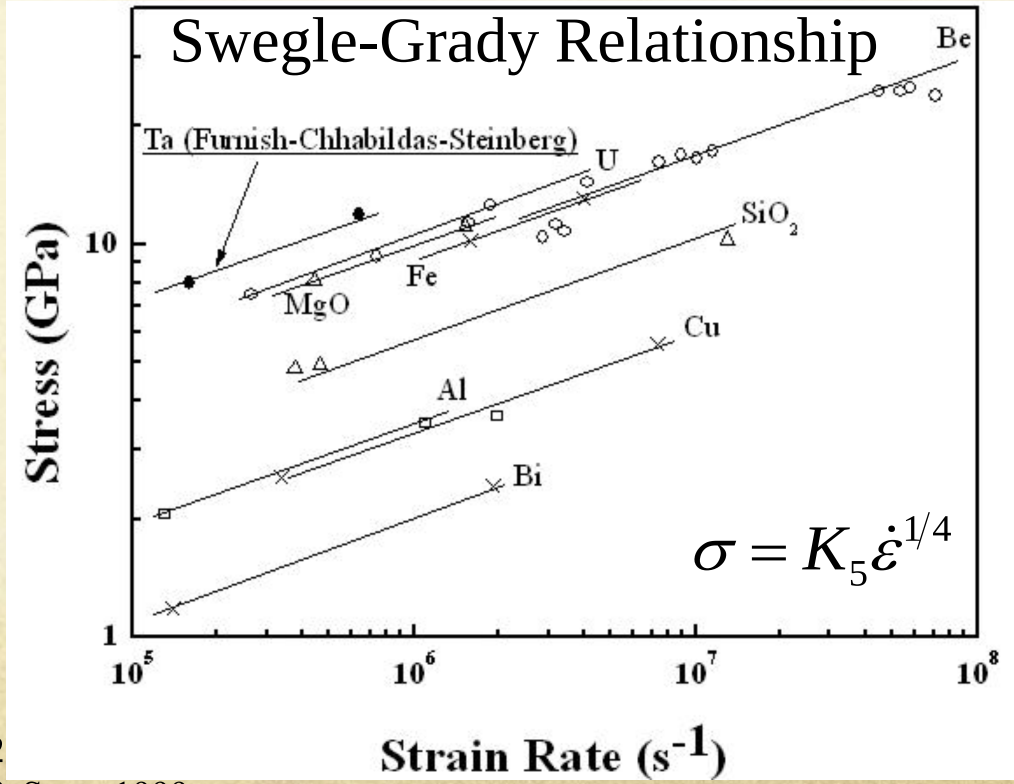
P. S. Follansbee, Metall. Mater. Tans. A, 41A (2010) 3080

Shock-Wave Deformation

Shock-Wave Deformation

- Shock-Wave region: strain rate over $10^5\ s^{-1}$
- Plastic wave propagation effects
- Shock front (simplified hydrodynamic approach) : discontinuity in pressure, temperature and density





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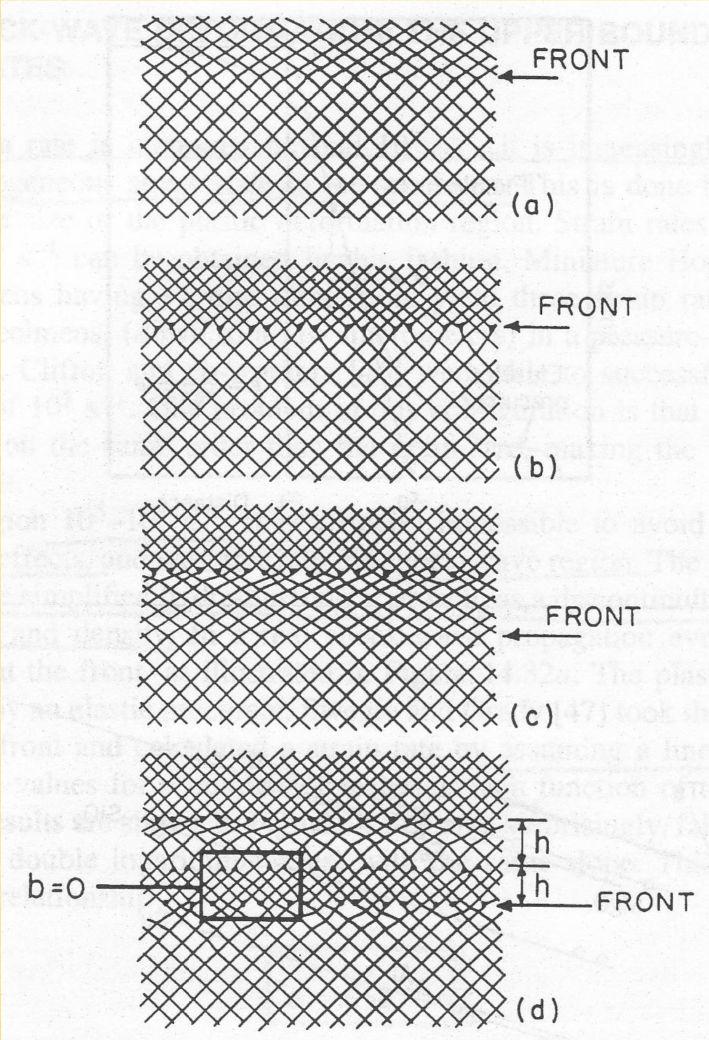
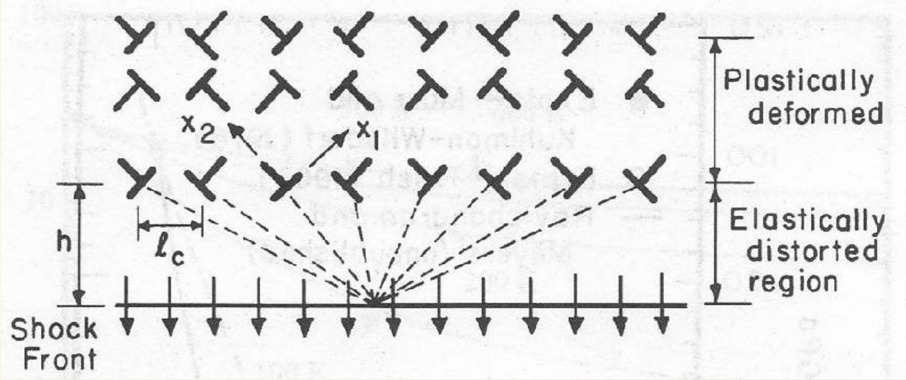
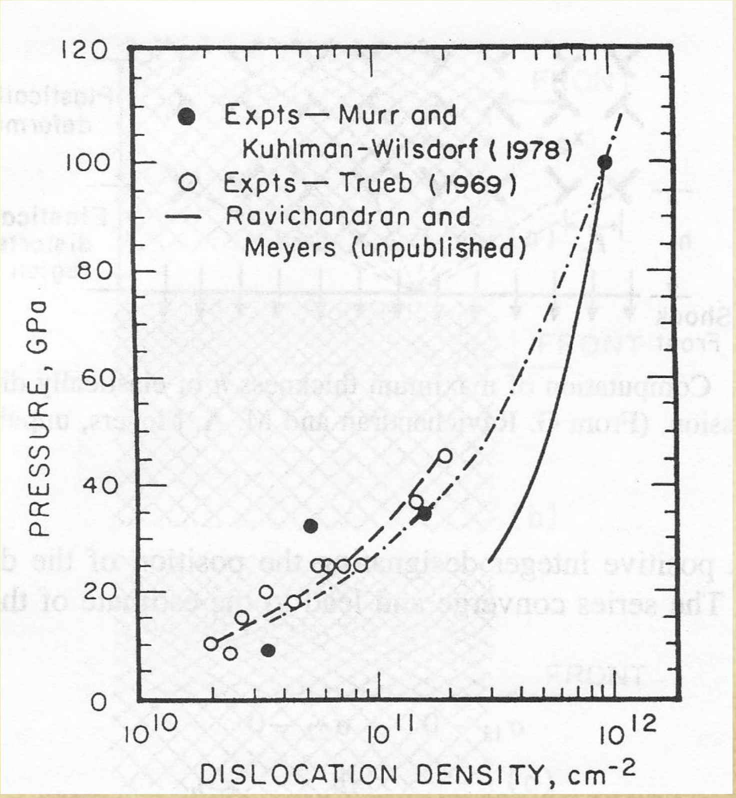
Smith Interface

- Meyers: dislocation generation mechanism at the shock front







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L. E. Murr and D. Kuhlmann-Wilsdorf, Acta Met., 26(1978) 847
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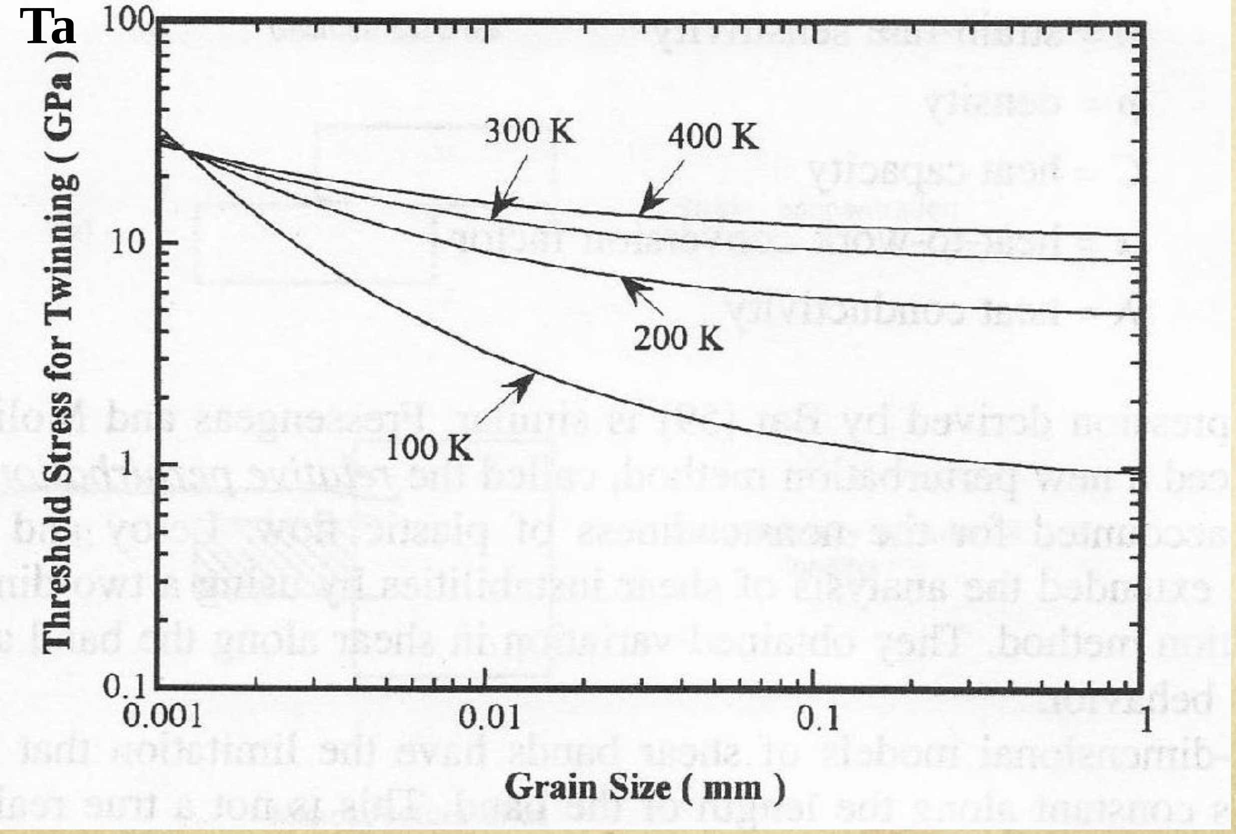
M. A. Meyers, in “Mechanics and Materials,” John Wiley & Sons, 1999

Grain Size Effect in Shock

- Apply Zerilli-Armstrong equations $\sigma^* = C_1 \exp\left(-C_3 T + C_4 T \ln \dot{\varepsilon}\right)$

  to Swegle-Grady Equation

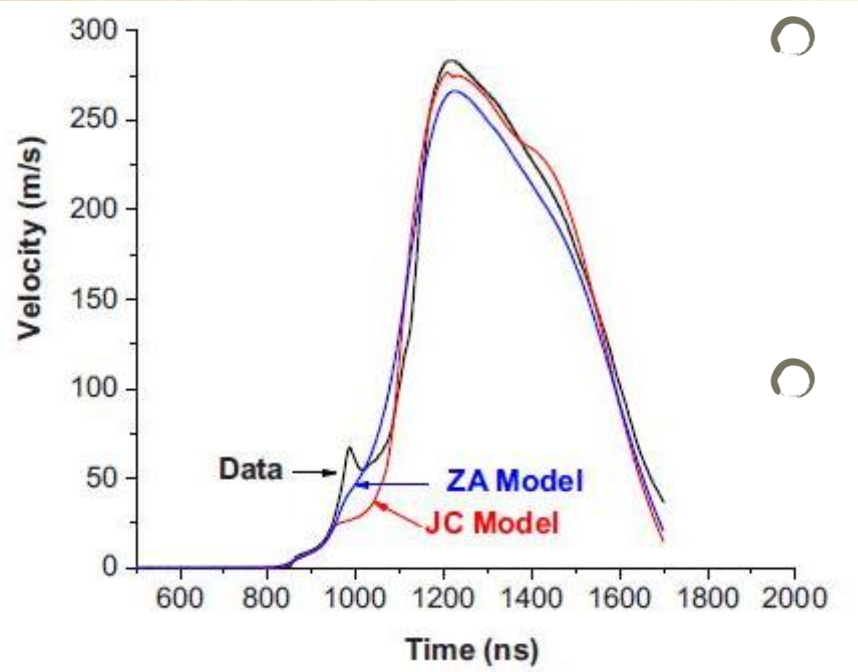
  Then $K'\left(K_5 \sigma_{sh}^4\right)^{1/(m+1)} e^{Q/(m+1)RT} - C_1 e^{-\left(C_3 - C_4 \ln K_5 \sigma_{sh}^4\right)T} + \left(k_T - k_S\right) D^{-(1/2)} - \sigma_G = 0$



M. A. Meyers, in “Mechanics and Materials,” John Wiley & Sons, 1999

Precursor Behavior Under High Pressure

- The amplitude of the elastic precursor is essentially independent of sample thickness
- Overstress viscoplastic model: used for a parametric study of dynamic material response under ramp and shock wave loading



- Plastic strain rate $\dot{\varepsilon}_{ij}^{p} = \dot{\varepsilon}^{p}\left(\frac{\sigma_{ij}^{'}}{\bar{\sigma}}\right)$

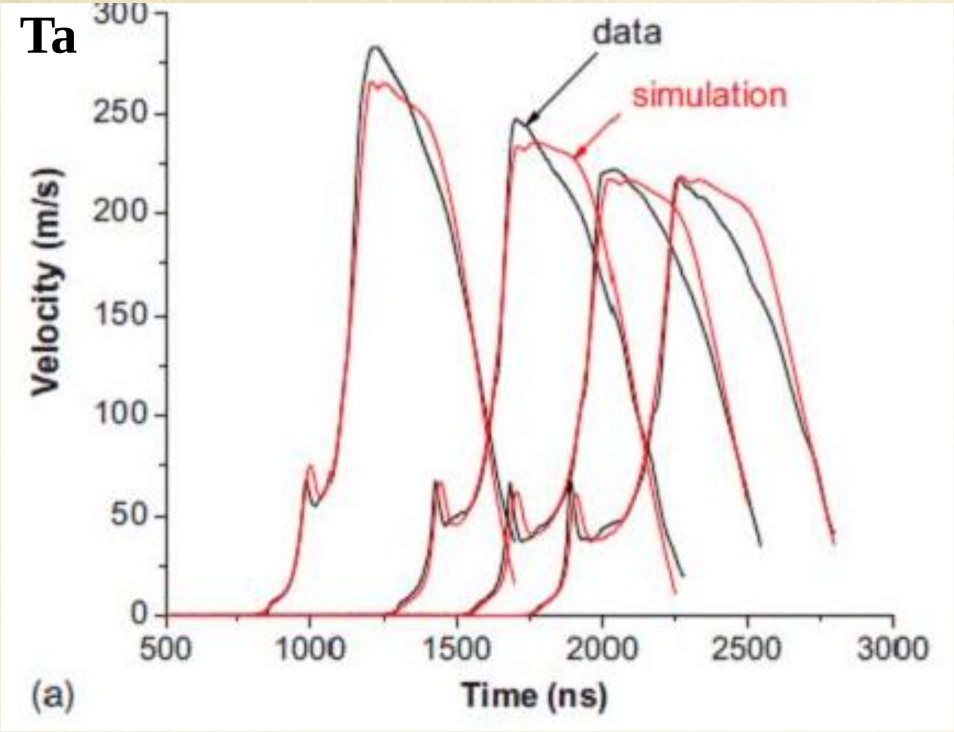
  effective plastic strain rate $\dot{\varepsilon}^{p} = A\left[\left(\bar{\sigma} - Y\right)/Y\right]^{n}$

  effective stress $\bar{\sigma}$, threshold strength Y
- Correlate $\dot{\varepsilon}^{p} = A\left[\left(\bar{\sigma} - Y\right)/Y\right]^{n}$ with Orowan equation and make A in the equation a function of dislocation density, which evolves with deformation history

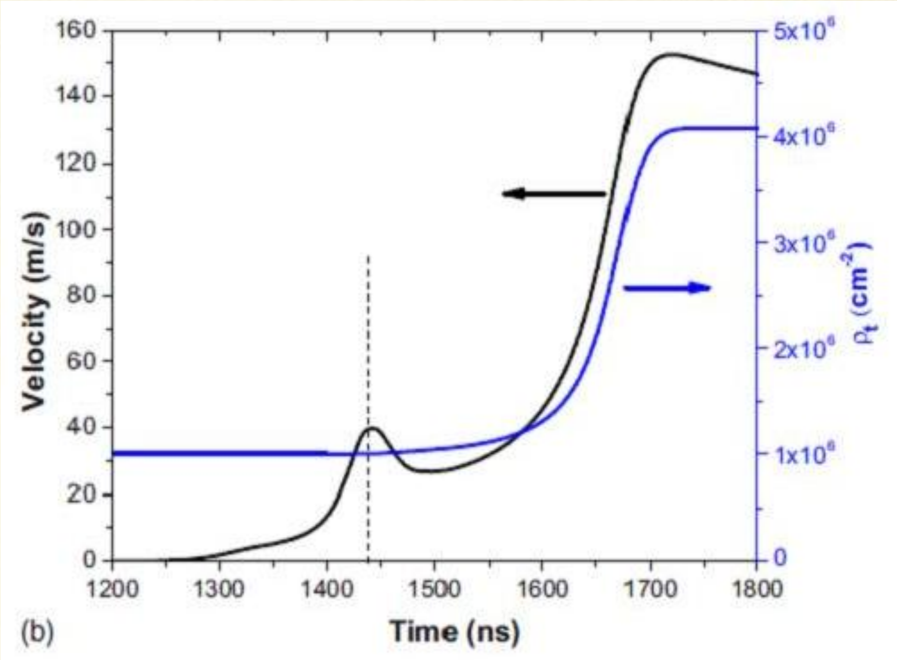
$$\dot{\varepsilon}^{p} = b\rho_{m}\bar{\upsilon} = b\rho_{m}B\left[\left(\bar{\sigma} - Y\right)/Y\right]^{n} = A\left[\left(\bar{\sigma} - Y\right)/Y\right]^{n}$$

J. L. Ding, J. R. Asay, and T. Ao, J. Appl. Phys. 107 (2010) 083508

Simulation Results . . . . .



- Total dislocation density:



- Some deviation at unloading part
  - Model does not capture precisely the detailed material behavior
  - Unloading occurs in the later time ➔ reflected wave and electromagnetic loading interaction

J. L. Ding, J. R. Asay, and T. Ao, J. Appl. Phys. 107 (2010) 083508

Summary and Conclusions

Summary and Conclusions

- Constitutive equation $\sigma = f\left(P, \ \varepsilon, \ \frac{d\varepsilon}{dt}, \ T, \ deformation \ \ history \right)$
  - connect the material features observed experimentally and numerical simulation
  - gain additional insight into the inelastic behavior, including material strength, under dynamic loading.
  - Stress as a function of strain, strain rate, temperature, grain size, impurity, and path history
- For shock-wave deformation:
  - Shock front model explain energy balance
  - Constitutive equation: Apply Zerilli-Armstrong equations to Swegle-Grady Equation

~ Thank you ~