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

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

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

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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

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

\[ \dot{\gamma} = \rho b \nu \]
Constitutive Equations: $\sigma = f(\varepsilon, \frac{d\varepsilon}{dt}, T, \text{deformation history})$

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

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
Dynamic Behavior
~ Dislocation Motion ~
BCC Slip Systems

Asymmetry in Dislocation Glide

- Core dislocation structure: $\frac{1}{2}[111]$ screw dislocation
- Maximum resolved shear stress plane (MRSSP) is $(\overline{1}01)$
Barriers to Dislocation Motion

Short-Range Barriers

**Rate Controlling Mechanisms**

<table>
<thead>
<tr>
<th></th>
<th>FCC</th>
<th>BCC</th>
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<tbody>
<tr>
<td>Dislocation Forests</td>
<td>$\nu^* \sim 100 - 1000 b^3$</td>
<td>Peierls-Nabarro Barrier</td>
</tr>
</tbody>
</table>

Dislocation Movement

- Peierls-Nabarro barrier
- Seeger kink-pair Mechanism
- Pinning

Dislocation Movement

BCC Molybdenum (Mo)

Uniaxial stress applied along the [001] axis

**Dislocation Dynamics**

### Regions of Dislocation Dynamics

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<td>Region I</td>
<td>$\nu \propto \tau^m e^{-Q/kT}$</td>
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<td>Region II</td>
<td>$\nu = \nu_0 \exp\left(-\frac{A}{\tau}\right)$</td>
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<tr>
<td>Region III</td>
<td>$\nu = \frac{kT}{h} K \exp\left(-\frac{\Delta H}{kT}\right) \exp\left[\frac{B(\tau_a - \tau_c)}{kT}\right]$ for iron</td>
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**Non-dimensional Parameters:**

- $m_I > 1$
- $m_{II} = 1$
- $m_{III} < 1$

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<tr>
<th>Authors</th>
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<tr>
<td>Johnston and Gilman</td>
<td>1959</td>
<td>$\nu \propto \tau^m e^{-Q/kT}$</td>
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<tr>
<td>Stein and Low</td>
<td>1960</td>
<td>$\nu = \nu_0 \exp\left(-\frac{A}{\tau}\right)$</td>
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<tr>
<td>Rohde and Pitt</td>
<td>1967</td>
<td>$\nu = \frac{kT}{h} K \exp\left(-\frac{\Delta H}{kT}\right) \exp\left[\frac{B(\tau_a - \tau_c)}{kT}\right]$ for iron</td>
</tr>
<tr>
<td>Gilman</td>
<td>1968</td>
<td>$\nu = \nu_v^<em>(1-e^{-\tau/\tau_v}) + \nu_d^</em> e^{-D/c}$</td>
</tr>
</tbody>
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Dislocation Behavior – Region I

- Physical based constitutive equation

- Apply Orowan equation: \( \dot{\gamma} = \dot{\gamma}_0 \exp \left[ -\frac{\Delta G}{kT} \right] \)

- At \( T_1 \): \( \Delta G = \Delta G_0 - \Delta G_1 \)

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

\[
 \tau = \tau_G + \frac{\Delta G_0}{V} + \frac{kT}{V} \ln \frac{\dot{\gamma}}{\dot{\gamma}_0}
\]
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
Zerilli-Armstrong Equation

- Two microstructurally based constitutive equations:
  - Activation area constant in BCC: \( \sigma^* = C_1 \exp(-C_3 T + C_4 T \ln \dot{\varepsilon}) \)
  - Hall-Petch equation: (D is the grain size) \( \sigma = \sigma_G + \sigma^* + kD^{-1/2} \)

- Zerilli-Armstrong equation for BCC metals:
  \[
  \sigma = \sigma_G + \sigma^* + kD^{-1/2} = \sigma_G + C_1 \exp(-C_3 T + C_4 T \ln \dot{\varepsilon}) + C_5 \varepsilon^n + kD^{-1/2}
  \]

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

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

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

Dislocation Behavior – Region II

Drag Regime

- Newtonian viscous behavior is assumed $f_v = B v$
- and using Orowan equation with orientation factor, $\sigma = \frac{4BM}{\rho b^2} \dot{\varepsilon}$
- Hirth and Lothe: viscosity coefficient from phonon viscosity

$$B = \frac{B_0}{1 - \left(\frac{\nu^2}{\nu_s^2}\right)} \approx \frac{bw}{10\nu_e} = \frac{b}{10\nu_e} \frac{3kT}{a^3}$$

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

- Thermal vibration
- Electron

Parameswaran, N. Urabe, and J. Weertman, JAP 43 (1972) 2982
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 \( \beta = \left( 1 - \frac{v^2}{v_s^2} \right)^{1/2} \)

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

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
- Sleeswyk:

A. H. Cottrell and B. A. Bilby, Phil. Mag. 42 (1951), 573
A. W. Sleeswyk, Acta Met. 10 (1962), 803
Mild Temperature Effect

- Dislocation Motion
- Twin Motion

Fe

**Graph:**
- True Stress (MPa) vs. Temperature (K)
- Data points for different temperatures and strain rates.
- Lines representing various data sets.

Constitutive Equation for Twinning

Consider dislocation pileup: (a high local stress is required)

Frank-Read or a Koehler source

Individual dislocation (Johnston and Gilman):

\[ \nu = A \tau^m e^{-Q/kT} \]

\[ \sigma_T = 2 \left( \frac{n^* L E}{2 A} \right)^{1/(m+1)} \hat{\varepsilon}^{1/(m+1)} e^{Q/(m+1)RT} = K' \hat{\varepsilon}^{1/(m+1)} e^{Q/(m+1)RT} \]

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Slip-Twinning Transition (MD)

- Screw dislocation in BCC iron (Fe)
- Atomic-sized kink
- Pinning points
- Twinning

Dynamic Behavior
~ Grain Size Effects ~
Grain Size Effect

- Hall-Petch-like Relationship: $\sigma_T = \sigma_0 + k_T d^{-1/2}$

- 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


Dynamic Behavior
~ Impurity Effects ~
Two-Obstacle Model

\[ \sigma = \sigma_a + \sigma_p + \sigma_i : \frac{\sigma}{\mu} = \frac{\sigma_a}{\mu} + S_p(\dot{\varepsilon}, T) \frac{\hat{\sigma}_p}{\mu_0} + S_i(\dot{\varepsilon}, T) \frac{\hat{\sigma}_i}{\mu_0} \]

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

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

- Strength of the obstacle vs. square root of the carbon concentration
Shock-Wave Deformation
Shock-Wave Deformation

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

M. A. Meyers, Scripta Met. 12 (1978) 21
Grain Size Effect in Shock

Apply Zerilli-Armstrong equations \( \sigma^* = C_1 \exp(-C_3T + C_4T \ln \dot{\varepsilon}) \)

to Swegle-Grady Equation

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

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 \( \dot{\varepsilon}^p = A[(\bar{\sigma} - Y)/Y]^n \)

- Effective stress \( \bar{\sigma} \), threshold strength \( Y \)

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

\[ \dot{\varepsilon}^p = b\rho_m \bar{\nu} = b\rho_m B[(\bar{\sigma} - Y)/Y]^n = A[(\bar{\sigma} - Y)/Y]^n \]

Simulation Results

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

Summary and Conclusions
Constitutive equation \( \sigma = f(P, \varepsilon, \frac{d\varepsilon}{dt}, T, \text{deformation history}) \)

- 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 ~