Thermally-activated dislocations: From individual movements through polycrystal and nanopolycrystal deformations to material dynamics calculations and highest rate tests

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Charles University, Prague, CZ, on 11 April, 2011
TOPICS

1. The flow stress dependence on strain rate, temperature and grain diameter
2. The Z-A equations for extension to dynamic computations
3. Extension of the pile-up based H-P equation to nanopolycrystals
Crystal grains, dislocations, slip, polycrystal plasticity/fracturing
Constitutive Equation Relations

The total range for creep, slip, twinning and cleavage dynamics:

\[ \varepsilon = \varepsilon \{ \Delta t, \sigma, D, T \} \rightarrow \sigma = \sigma \{(d\varepsilon/dt), T, \ell^{-1/2}\} \]

1. Thermal activation - strain rate analysis, TASRA, \((d\varepsilon/dt) = (d\varepsilon/dt)\{T, \tau_{Th}\}\):
   
   thus \((\partial\tau_{th}/\partial T)_{\ln[d\varepsilon/dt]}(\partial T/\partial \ln[d\varepsilon/dt])_{\tau_{Th}}(\partial \ln[d\varepsilon/dt]/\partial \tau_{Th})_T = -1.0\)
   
   and \((d\varepsilon/dt) = (d\varepsilon/dt)_0 \exp\{-(G_0 - \int v^* d\tau_{Th})/k_BT\}\), with \(v^* = A^*b\),
   
   and \(v^* = W_0/\tau_{Th}\) and \(\tau_{Th} = \tau - (\tau_G + k_{Se} \ell^{-1/2})\).

2. The Hall-Petch microstructural stress intensities, “k”s:

   For a circular pile-up: \(n(\tau - \tau_{0\varepsilon}) = m^*\tau_C\) and \(n = 2\alpha(\tau - \tau_{0\varepsilon})\ell/\pi Gb\)
   
   thus \(\sigma = m_T[(\tau_G + \tau_{Th}) + (\pi m^* Gb \tau_C/2\alpha)^{1/2} \ell^{-1/2}] = \sigma_{0\varepsilon} + k_{\varepsilon} \ell^{-1/2}\)
   
   and \(k_{Al} < k_{Cu} < k_{Mg} << k_{\alpha-Fe}\) with \(k_{\varepsilon} < k_{y.p.} << k_T \sim k_C << K_{IC} = \sigma(\pi c)^{1/2}\)
   
   with \(c\) and \(\ell\) being analogous in comparison with the fracture mechanics \(K_{IC}\).
First, thermal activation, and a critical role for the dislocation activation volume: 

\[ v^* = bA^* = kT \left[ \frac{\partial \ln(d\varepsilon/dt)}{\partial \tau_{Th}} \right]_T \]

Z-A Constitutive Equations

\[ \frac{d\varepsilon}{dt} = \frac{1}{m} \rho b v \]

\[ v = v_0 \exp[-(G_0 - \int A^* b d\tau_{Th}) / k_B T] \] and \[ A^* b = W_0 / \tau_{Th} \]

Computational (Z-A) equations:

\[ \sigma = \sigma_G + B \exp[-\beta T] + \]

\[ B_0 [\varepsilon_r (1 - \exp\{- \varepsilon / \varepsilon_r\})]^{1/2} \exp[-\alpha T] + k \varepsilon^{1/2} \exp[-\alpha T] \]

in which

\[ (\beta, \alpha) = (\beta_0, \alpha_0) - (\beta_1, \alpha_1) \ln(d\varepsilon/dt) \]

bcc case: \[ \alpha = \alpha_0 = \alpha_1 = 0 \]

fcc case: \[ B = \beta = \beta_0 = \beta_1 = 0 \]

Z-A and J-C stress-strain curves for Cu

\( B_0 = 890 \text{ MPa}, \alpha_0 = 0.0028 \text{ K}^{-1}, \alpha_1 = 0.000115 \text{ K}^{-1}, (\varepsilon/\varepsilon_r) < 1.0, k_e = 5 \text{ MPa.mm}^{1/2}, \sigma_G + k_e \ell^{-1/2} = 65 \text{ MPa} \)

Taylor Cu cylinder impact test result

\[ 0 < \varepsilon_t < 1.5, \ 0 < (d\varepsilon_t/dt) < 10^5 \text{ s}^{-1}, \ 300 < T < 600 \text{ K} \]

Cu extensions on tensile impact

Impacted Cu and Mild Steel Tensile Extensions

Original Taylor-type cylinder impact test result on mild steel

SHPB twinning measurements compared to Z-A slip calculations

Armco iron Taylor impact test involving twinning and slip

The H-P polycrystal \((\ell^{-1/2})\) aspect of \(\sigma = \sigma\{T, (d\varepsilon/dt), \ell^{-1/2}\}\)

\[
\sigma = m[(\tau_G + \tau_{Th}) + (\pi m^* Gb\tau_C / 2\alpha)^{1/2}]\ell^{-1/2} = \sigma_{0\varepsilon} + k_{\varepsilon}\ell^{-1/2}
\]

1. A strong influence of grain diameter particularly enters if \(m, m^*\) and/or \(\tau_C\) are/is large.

2. For bcc metals and alloys, \(\tau_C\) is generally so large as to be athermal because of interstitial-caused yield point behavior.

3. For hcp metals, \(m, m^*, \) and \(\tau_C\) are relatively large but \(\tau_C = (\tau_{CG} + \tau_{CTh})\) is thermally-dependent for prism or pyramidal slip.

4. For pure fcc metals, \(\tau_C\) is determined by the cross-slip shear stress, \(\tau_{III}\), that is thermally dependent.

A Hall-Petch dependence for iron and steel materials

Mg: $\sigma_0$ matched with $\tau_{(0001)}$ and $k_{\varepsilon}^2$, with $\tau_{(1-100)}$

Cu: $T$ and $(d\varepsilon/dt)$ dependencies for $k^2$ and $\tau_{III}$

\[ \beta \sim 0.005 \text{ K}^{-1} \text{ as compared with } \beta_0 = 0.0028 \text{ K}^{-1} \text{ and } \beta_1 \sim 0.002 \text{ K}^{-1} \text{ as compared with } \beta_1 = 0.000115 \text{ K}^{-1} \]

An H-P type dependence for the reciprocal activation volume

1. Consider the strain rate dependence contained in both H-P equation terms:

$$\left[ \frac{\partial \sigma}{\partial \ln (d\varepsilon/dt)} \right]_T = \left[ \frac{\partial (\sigma_0 + k_{\varepsilon} \ell^{-1/2})}{\partial \ln (d\varepsilon/dt)} \right]_T$$

2. There are two strain rate terms to deal with

$$\left[ \frac{kT}{v^*} \right] = \left[ \frac{\partial (m \tau_{0T})}{\partial \ln (d\varepsilon/dt)} \right]_T +$$

$$\left[ \frac{\partial (m \{\pi m^* Gb_C/2\alpha\}^{1/2} \ell^{-1/2})}{\partial \ln (d\varepsilon/dt)} \right]_T$$

3. Thus

$$v^*{-1} = v^*_o^{-1} + \left( k_{\varepsilon}/2mCv^*_C \right) \ell^{-1/2}$$

4. At small $\varepsilon$, $(\tau_{CTh} + \tau_G)v^*_C \sim \tau_{CTh}v^*_C \sim W_0$, and so an H-P type dependence is obtained for the polycrystal $v^*{-1}$
An H-P type $v^{-1}$ dependence for polycrystal Zn

Mg: $v^{-1}$ on a log/log basis for a large range in $\ell$

Cu: \( v^{-1} \) on an H-P basis from \( \sigma_{0\varepsilon} \) and \( k_\varepsilon \) component dependencies

Cu: An H-P dependence for $v^{-1}$ on a log/log basis

Zn: H-P results on a log/log scale

Zn: $v^{-1}$ aspects of transition from H-P strengthening

Newest high rate deformation concerns initiated by SHPB pre-shock indication of dislocation generations

Nanoscale dislocation generation at a propagating shock front

\[
\sigma = \left( \frac{2G_0}{v_0^*} \right) - \left( \frac{2kT}{v_0^*} \right) \ln \left[ \frac{(d\varepsilon/dt)_0}{(d\varepsilon/dt)} \right]
\]

Shocked Armco iron at different grain sizes and strain rates

Plastic front propagation by nanoscale twinning

Shockless isentropic compression experiments (ICEs)

The resident dislocation density is required to “carry the load”, and because $\rho_N$ is low, $\nu_N$ is so high as to be controlled by “drag”!

$$\sigma_{Th} = \left(1 - \left[c(\text{d}\varepsilon/\text{d}t)/\beta_1 \sigma_{Th}\right]^{-\beta_1 T}\right) [B \exp(-\beta T)]$$

in which

$$c = c_0 m^2 \beta_1 / \rho b^2 \quad \text{and} \quad b\tau_{TH} = c_0 \nu.$$

At high $\text{d}\varepsilon/\text{d}t$:

$$\sigma_{Th} = (c_0 m^2 / \rho b^2)(\text{d}\varepsilon/\text{d}t)$$

Drag-controlled shockless ICE results for copper

SUMMARY

1. Experimental evidence has been presented for a thermally-activated, dislocation mechanics based, constitutive equation description of temperature, strain rate and grain diameter influences on polycrystal plasticity.

2. Important extension has been to the nanoscale-dimensioned properties of a number of engineering materials for which the size of the dislocation defect structures become comparable to the crystal lattice dimensions.

3. There is important extension to mechanical property influences of material deformations occurring at the limit of high rate deformations, for example, connecting with propagating shock wave fronts and their own nanoscale structures.