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

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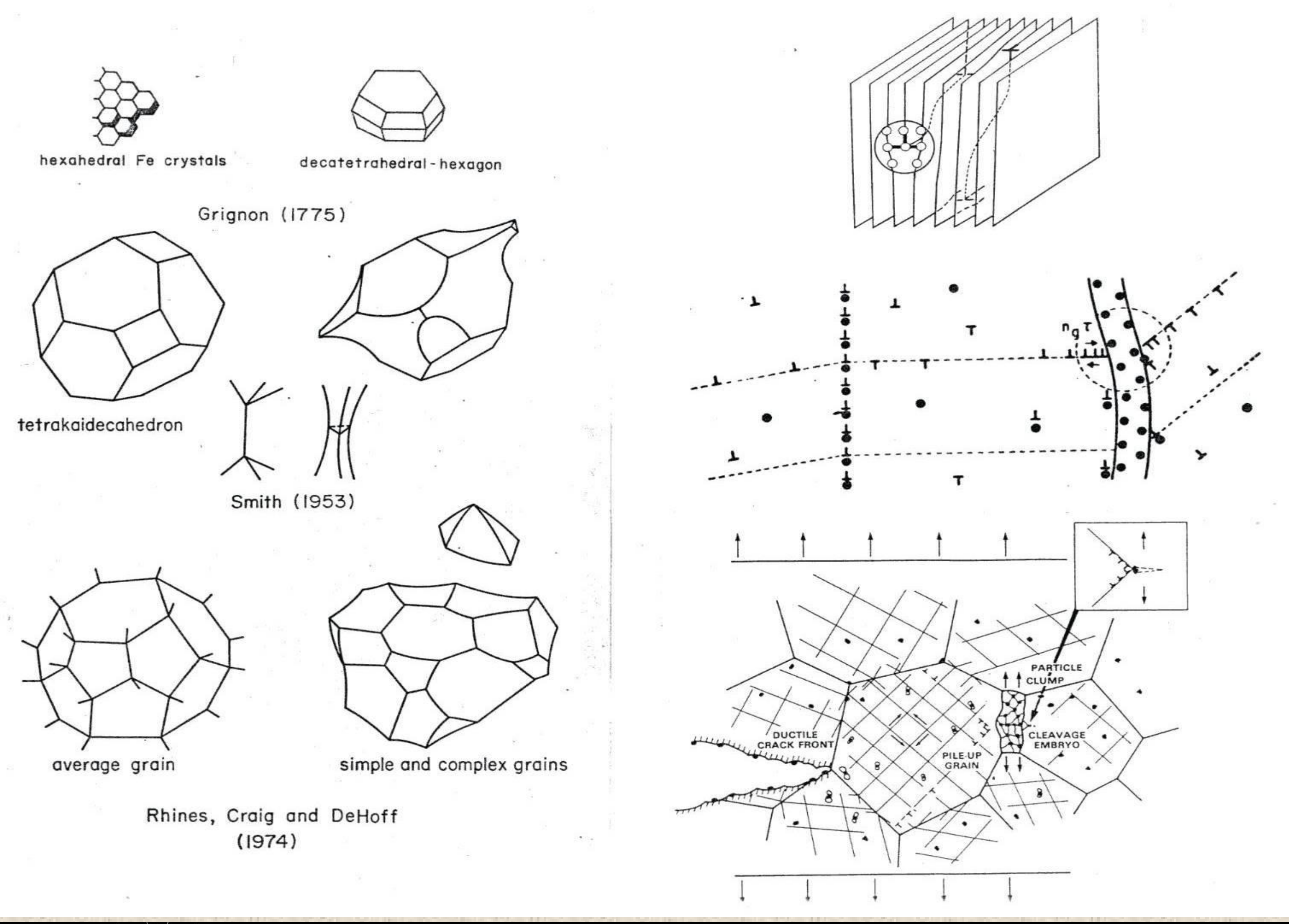
# TOPICS

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 $(\partial\tau_{th}/\partial T)_{\mathbf{ln}[d\varepsilon/dt]}(\partial T/\partial \mathbf{ln}[d\varepsilon/dt])_{\tau Th}\,(\partial \mathbf{ln}[d\varepsilon/dt]/\partial\tau_{Th})_T = -1.0$

   and $(d\varepsilon/dt) = (d\varepsilon/dt)_0 \mathbf{exp}\{-(G_0 - \int v^* d\tau_{Th})/k_B T\}$, with $v^* = A^* b$,

   and $v^* = W_0/\tau_{Th}$ and $\tau_{Th} = \tau - (\tau_G + k_{S\varepsilon}\ell^{-1/2})$.

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

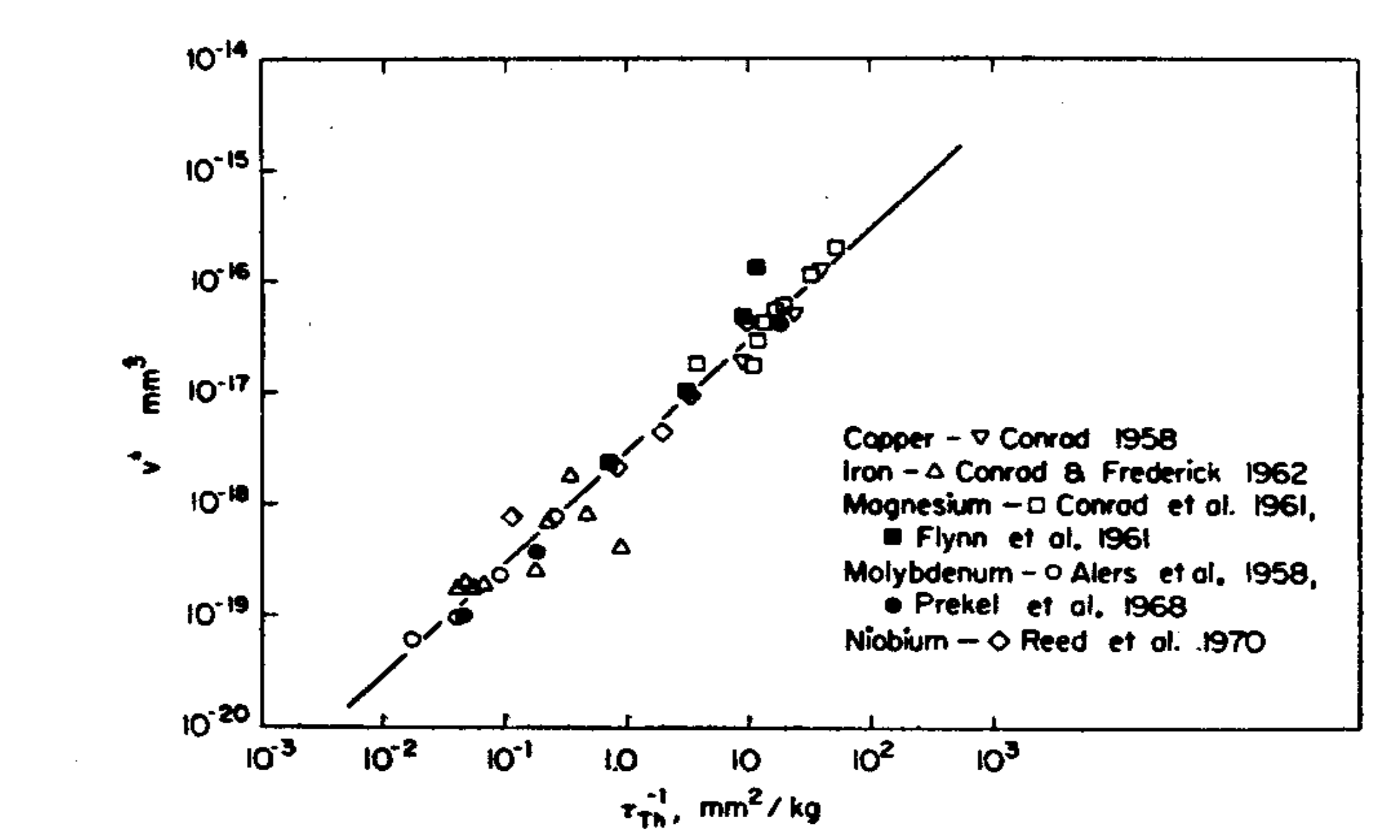
   For a circular pile-up; $n(\tau - \tau_{0\varepsilon}) = m^*\tau_C$ and $n = 2\alpha(\tau - \tau_{0\varepsilon})\ell/\pi G b$

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

   and $k_{Al} < k_{Cu} < k_{Mg} << k_{\alpha\text{-}Fe}$ 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: $v^* = bA^* = kT[\partial \mathbf{ln}(d\varepsilon/dt)/\partial \boldsymbol{\tau}_{Th}]_T$




R.W. Armstrong, *(Indian) J. Sci. Indust. Res.*, **32**, 591-598 (1973)

# Z-A Constitutive Equations

$$(d\varepsilon/dt) = (1/m)\rho b\nu$$

$$\nu = \nu_0\mathbf{exp}[-(G_0 - \int A^*bd\tau_{Th})/k_BT] \text{ and } A^*b = W_0/\tau_{Th}$$

Computational (Z-A) equations:

$$\sigma = \sigma_G + B\mathbf{exp}[-\beta T] +$$

$$B_0[\varepsilon_r(1 - \mathbf{exp}\{-\varepsilon/\varepsilon_r\})]^{1/2}\mathbf{exp}[-\alpha T] + k_\varepsilon \ell^{-1/2}$$

in which

$$(\beta,\alpha) = (\beta_0,\alpha_0) - (\beta_1,\alpha_1)\mathbf{ln}(d\varepsilon/dt)$$

bcc case: $\alpha = \alpha_0 = \alpha_1 = 0$

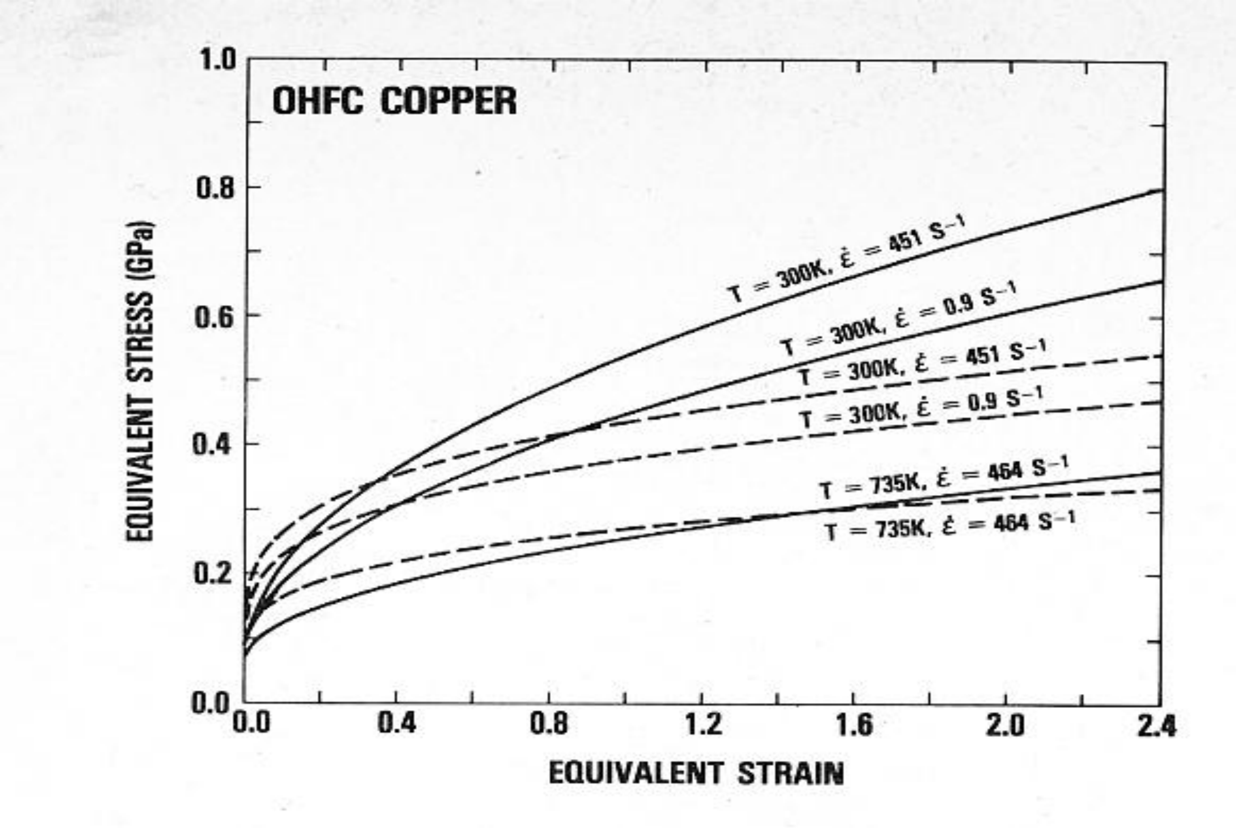
fcc case: $B = \beta = \beta_0 = \beta_1 = 0$

F.J. Zerilli and R.W. Armstrong, *J. Appl. Phys.* **61**, 1816-1825 (1987)

F.J. Zerilli and R.W. Armstrong, *J. Appl. Phys.* **68**, 1580-1591 (1990)

F.J. Zerilli, *Metall. Mater. Trans. A*, **35A**, 2547-2555 (2004)

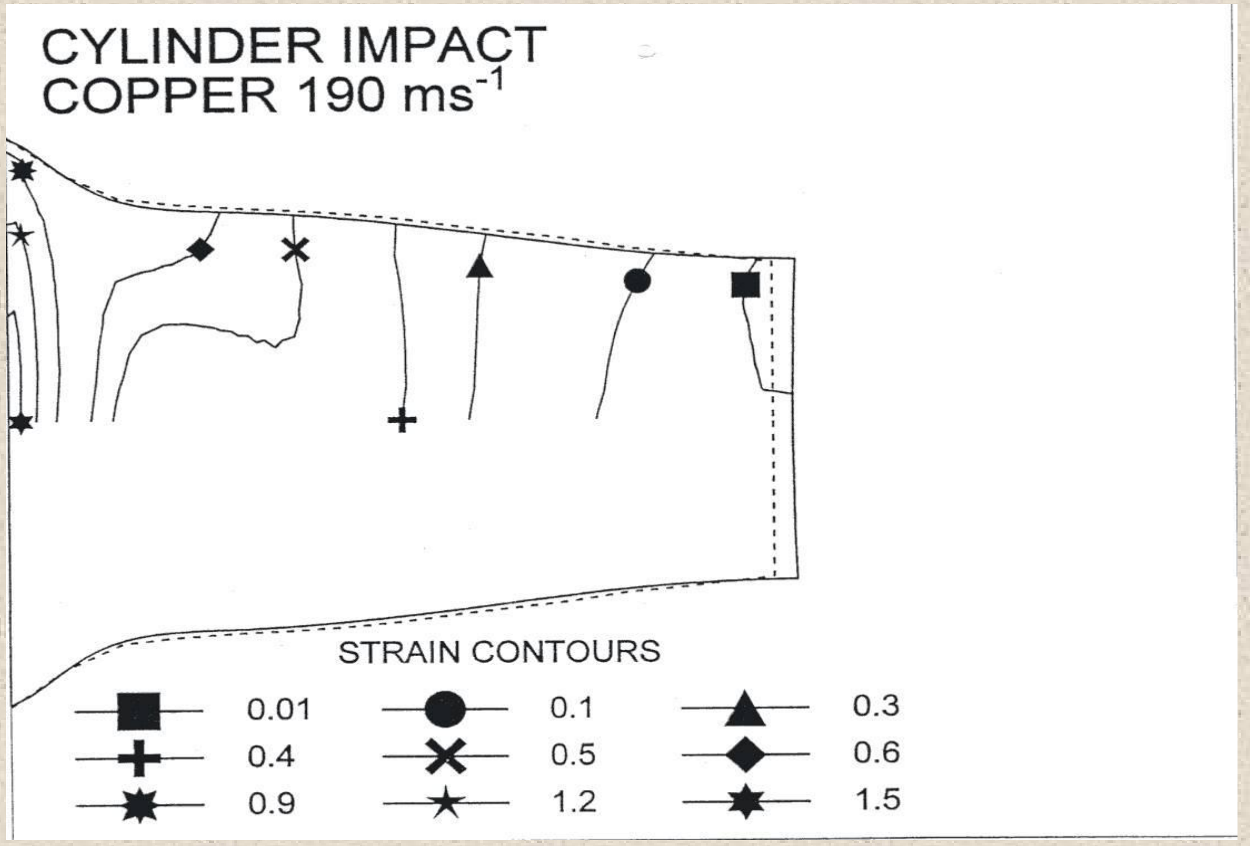
# Z-A and J-C stress-strain curves for Cu




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

F.J. Zerilli and R.W. Armstrong, *J. Appl. Phys.* **61**, [5], 1816-1826 (1987); G.R. Johnson and W.H. Cook, *Eng. Fract. Mech.*, **21**, 31-48 (1985)

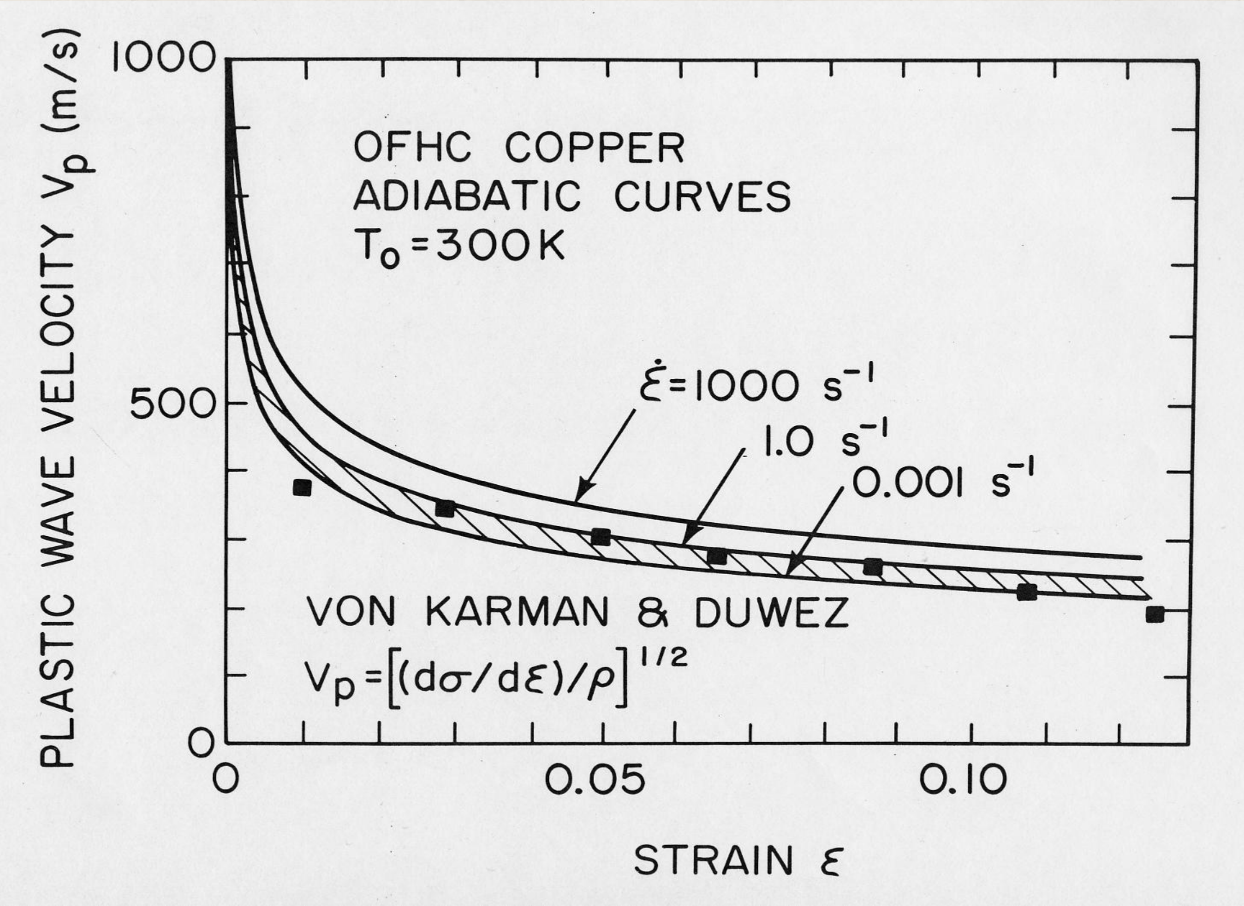
# Taylor Cu cylinder impact test result




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

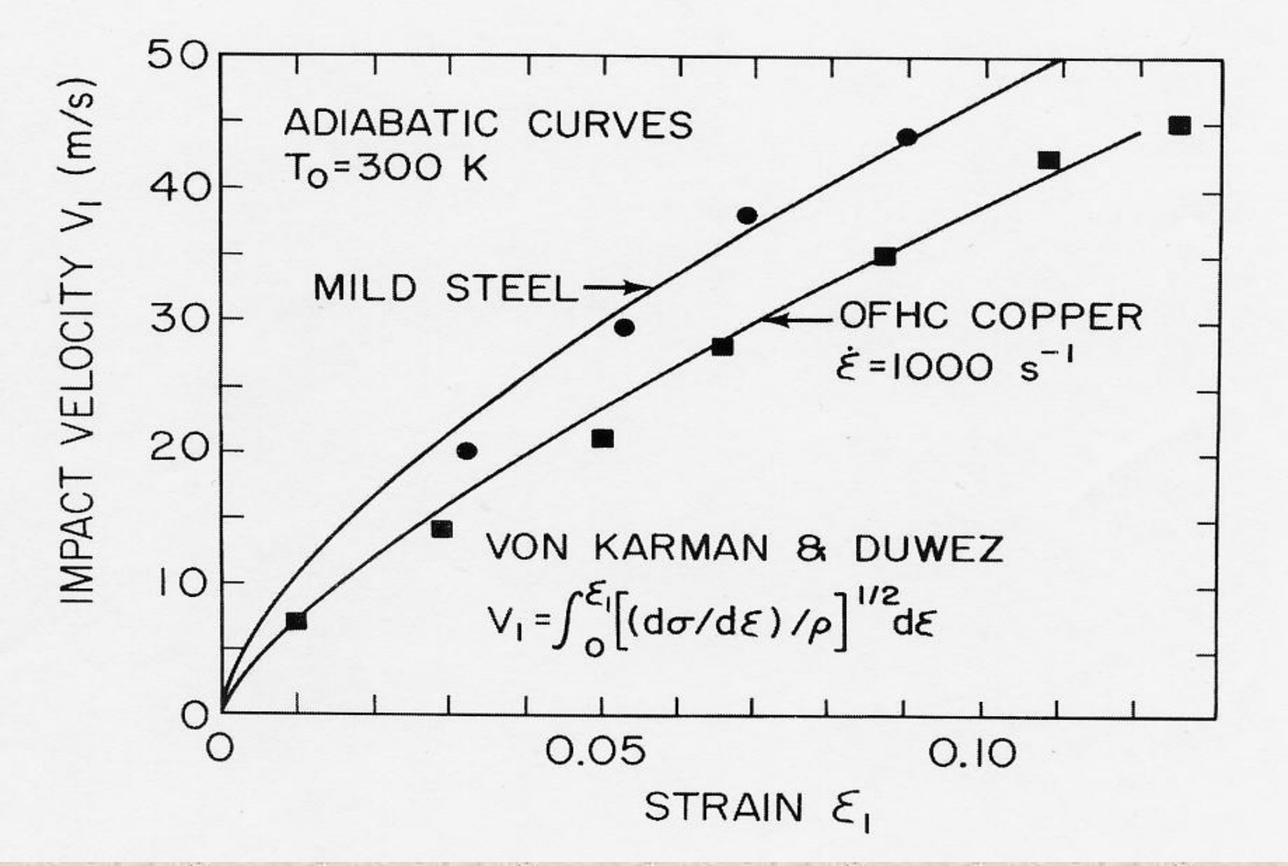
F.J. Zerilli and R.W. Armstrong, *J. Appl. Phys.*, **61**, [5], 1816-1825 (1987);
G.R. Johnson and W.H. Cook, *Eng. Fract. Mech.*, **21**, 31-48 (1985)

# Cu extensions on tensile impact



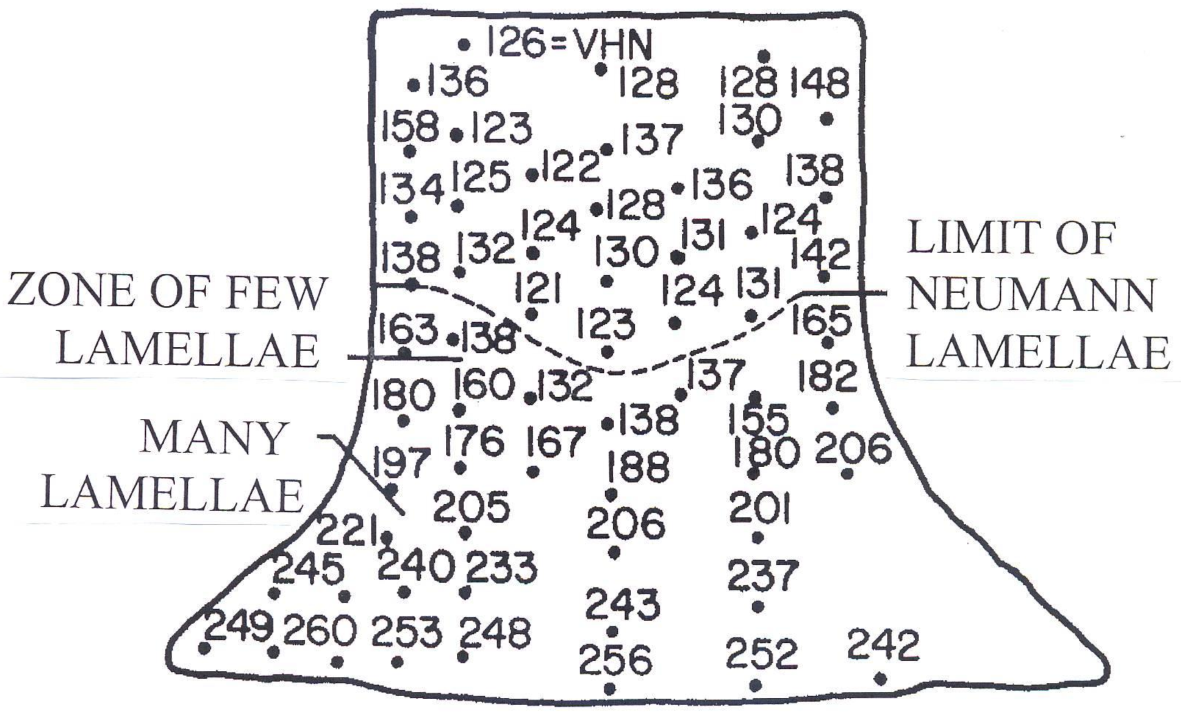

R.W. Armstrong and F.J. Zerilli, *J. Phys. Fr Colloq.*, **49** , (C3) , 529-534 (1988); after T. Von Karman and P. Duwez, *J. Appl. Phys.*, **21**, 987-994 (1950).

# Impacted Cu and Mild Steel Tensile Extensions




R.W. Armstrong and F.J. Zerilli, *J. Phys. Fr. Colloq.*, **49**, (C3), 529-534 (1988); after T. Von Karman and P. Duwez, *J. Appl. Phys.*, **21**, 987-994 (1950

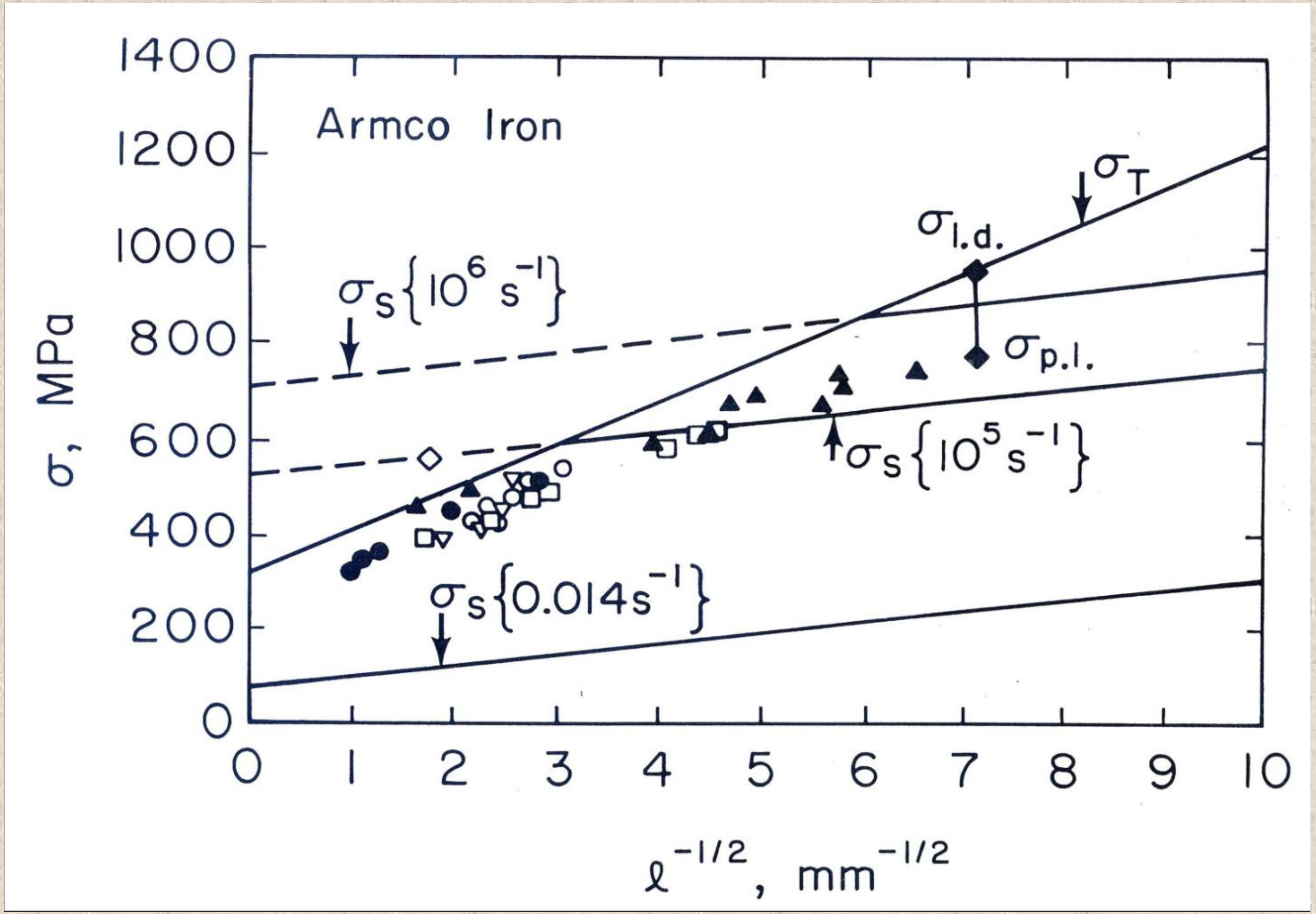
# Original Taylor-type cylinder impact test result on mild steel




MILD STEEL CYLINDER. IMPACT VELOCITY 338 m/s

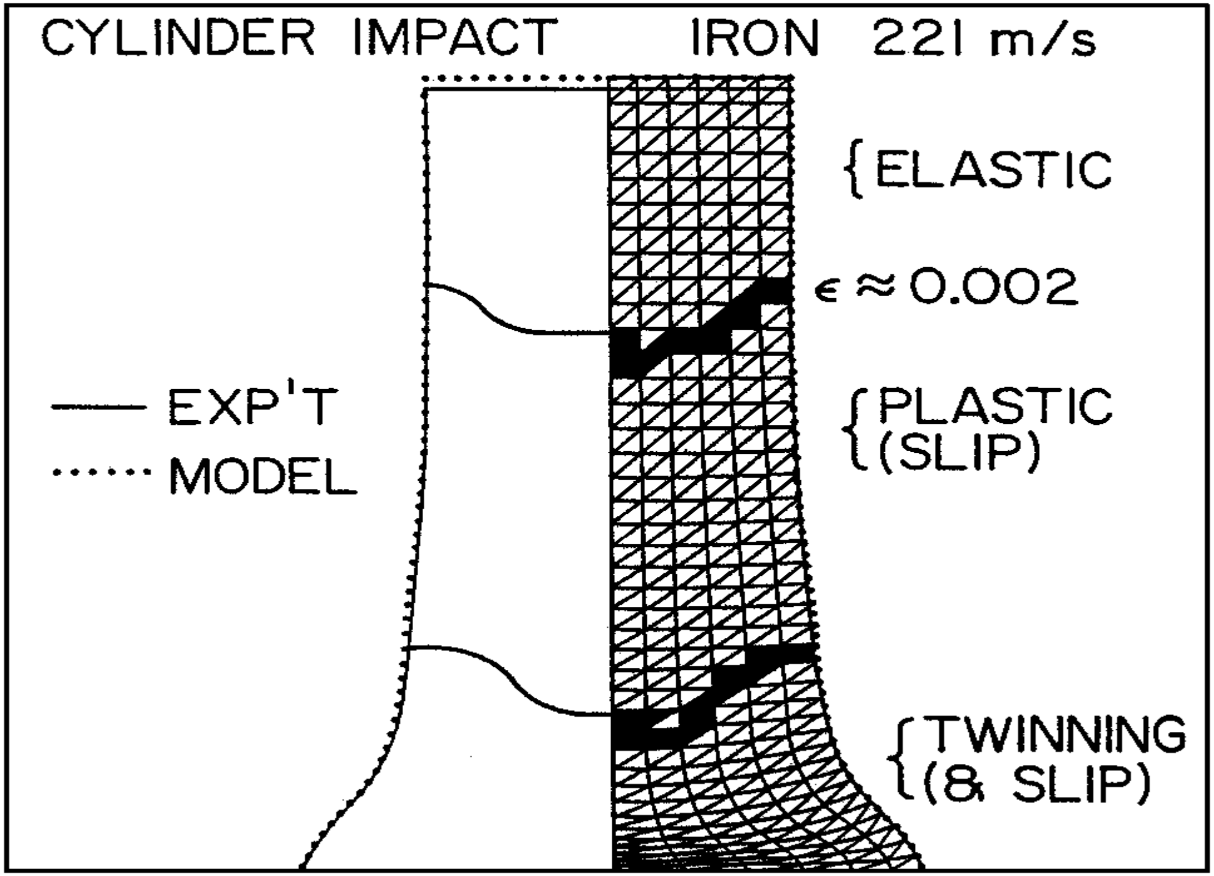
W.E. Carrington and M.L.V. Gaylor, Proc. Roy. Soc. London A, 194A, 323-331 (1948)

# SHPB twinning measurements compared to Z-A slip calculations




R.W.Armstrong and F.J. Zerilli, *J. Phys. Fr. Colloq.*, **49**, (C3), 529-534 (1988)

# Armco iron Taylor impact test involving twinning and slip




F.J. Zerilli and R.W. Armstrong, *Shock Compression of Condensed Matter*, edited by S.C. Schmidt and N.C. Holmes (Elsevier Sci. Publ. B.V., NY, 1988) pp. 273-277.

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

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

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

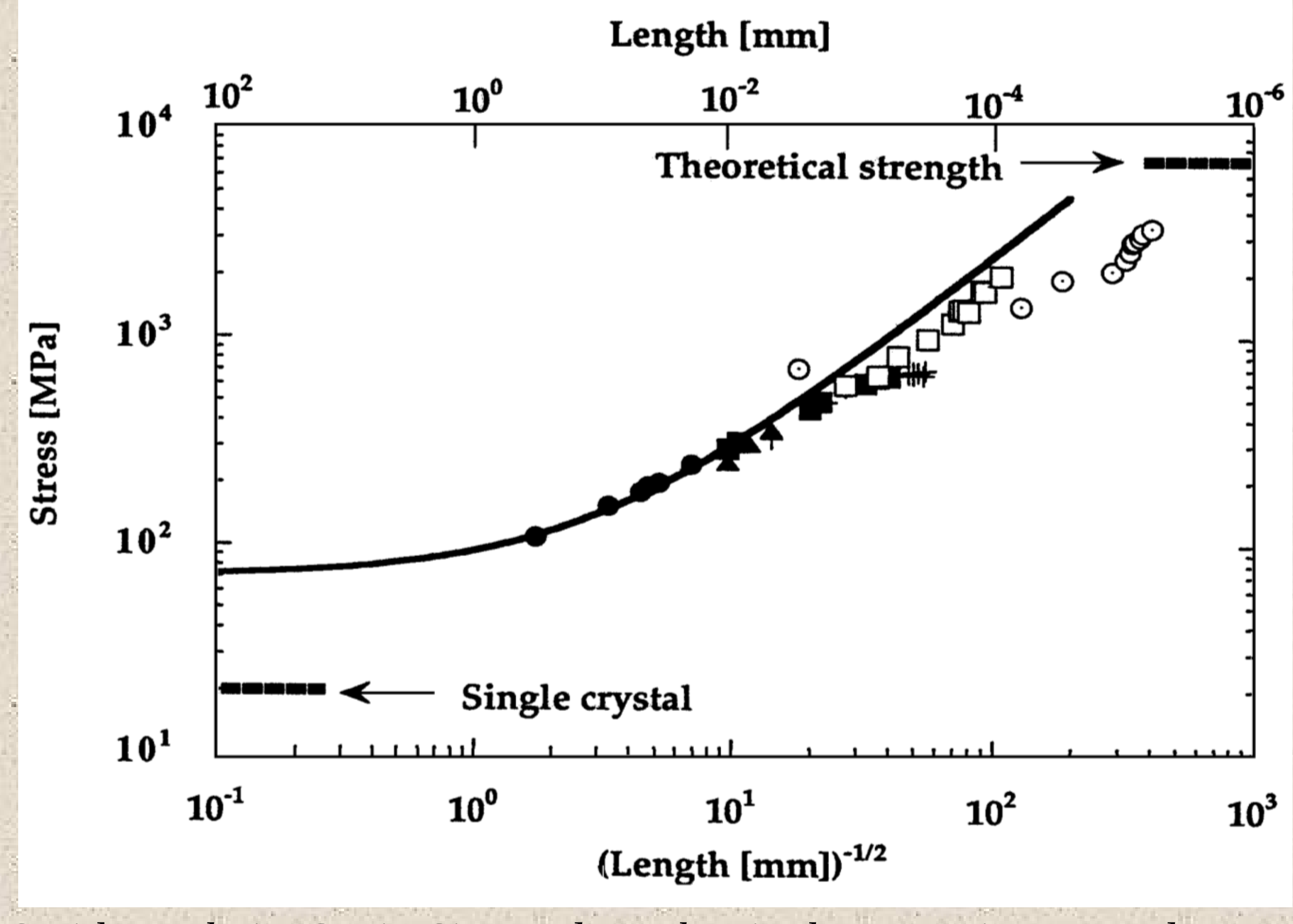
**2**. For bcc metals and alloys, $\tau_C$ is generally so large as to be athermal because of interstitial-caused yield point behavior.

**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.

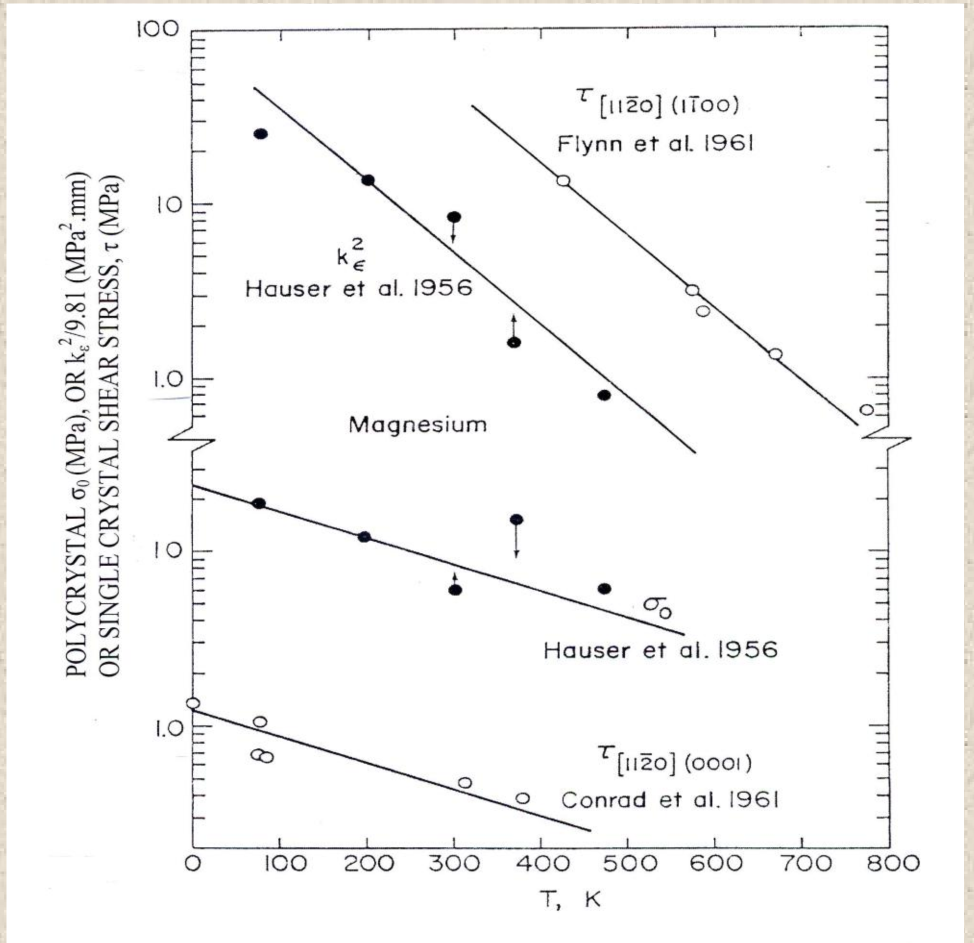
R.W. Armstrong, I. Codd, R.M. Douthwaite and N.J. Petch, *Philos. Mag.*, **7**, 45-53 (1962).

# A Hall-Petch dependence for iron and steel materials



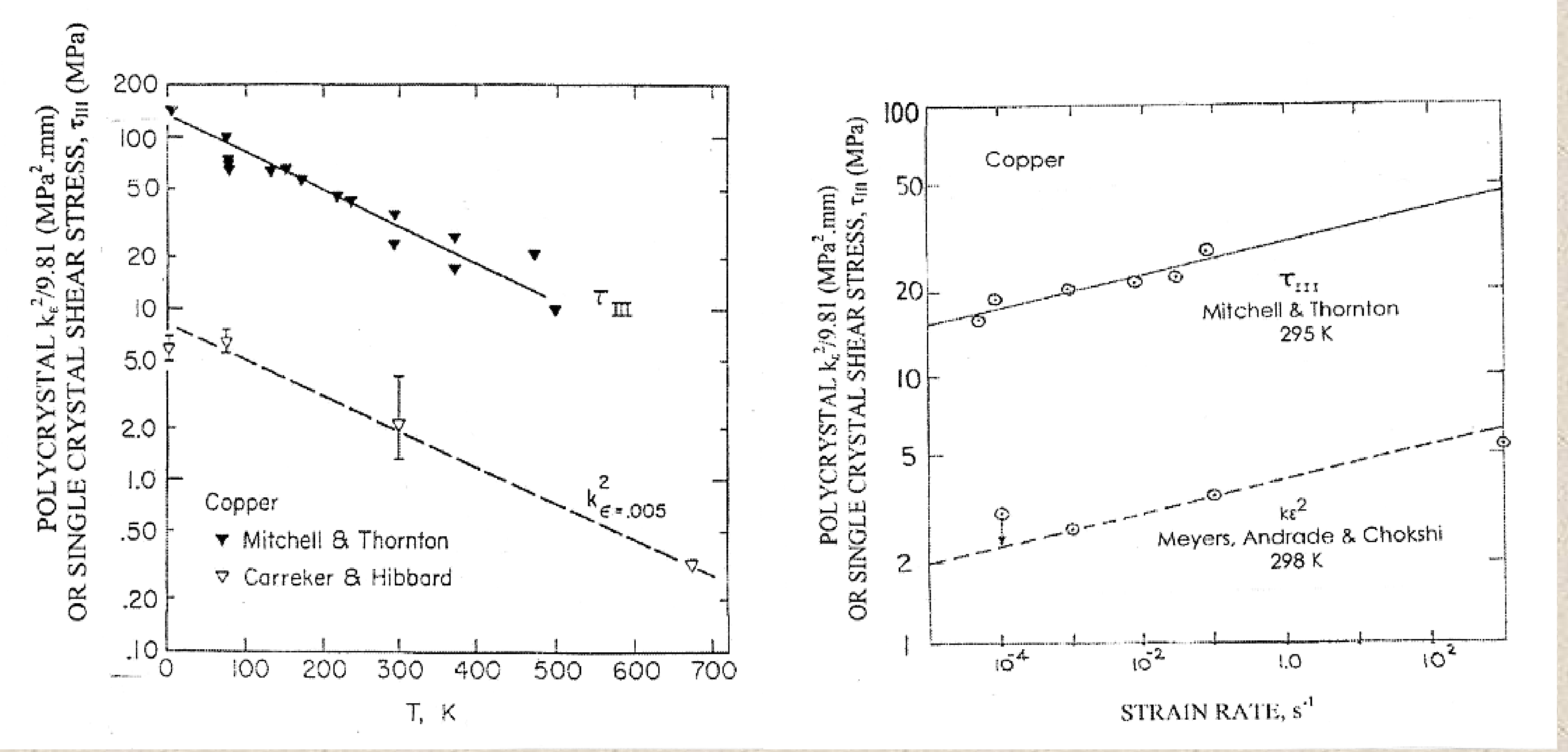

T.R. Smith *et al.*, in *Grain Size and Mechanical Properties – Fundamentals and Applications*, edited by M.A. Otooni et al., *Mater. Res. Soc.*, **362**, 31-37 (1995)

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




R.W. Armstrong, *Acta Metall*., **16**, 347-355 (1968)

# Cu: *T* and *(dε/dt)* dependencies for $k^2$ and $\tau_{III}$




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

R.W. Armstrong, *Trans Indian Inst. Met.*, **50**, 521-531 (1997)

An H-P type dependence for the reciprocal activation volume

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

$$[\partial\sigma_\varepsilon/\partial\mathbf{ln}(d\varepsilon/dt)]_T = [\partial(\sigma_{0\varepsilon} + k_\varepsilon\ell^{-1/2})/\partial\mathbf{ln}(d\varepsilon/dt)]_T$$

2. There are two strain rate terms to deal with

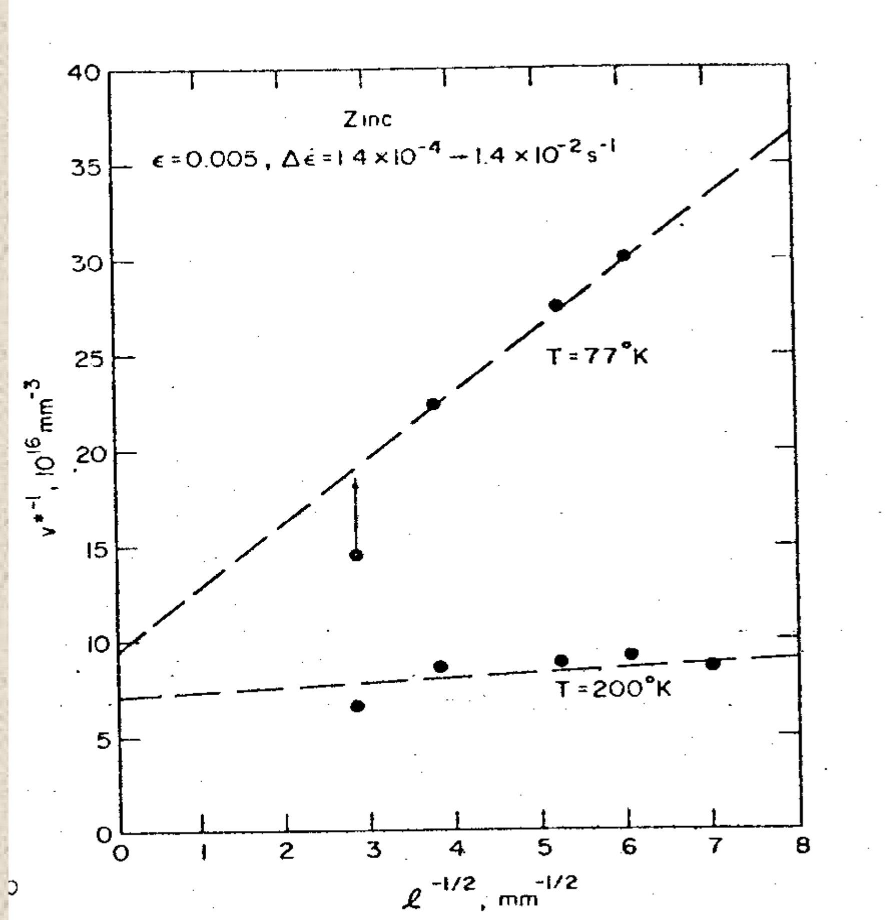
$$[kT/v^*] = [\partial(m\tau_{0Th})/\partial\mathbf{ln}(d\varepsilon/dt)]_T + [\partial(m\{\pi m^* Gb\tau_C/2\alpha\}^{1/2}\ell^{-1/2})/\partial\mathbf{ln}(d\varepsilon/dt)]_T$$

3. Thus

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

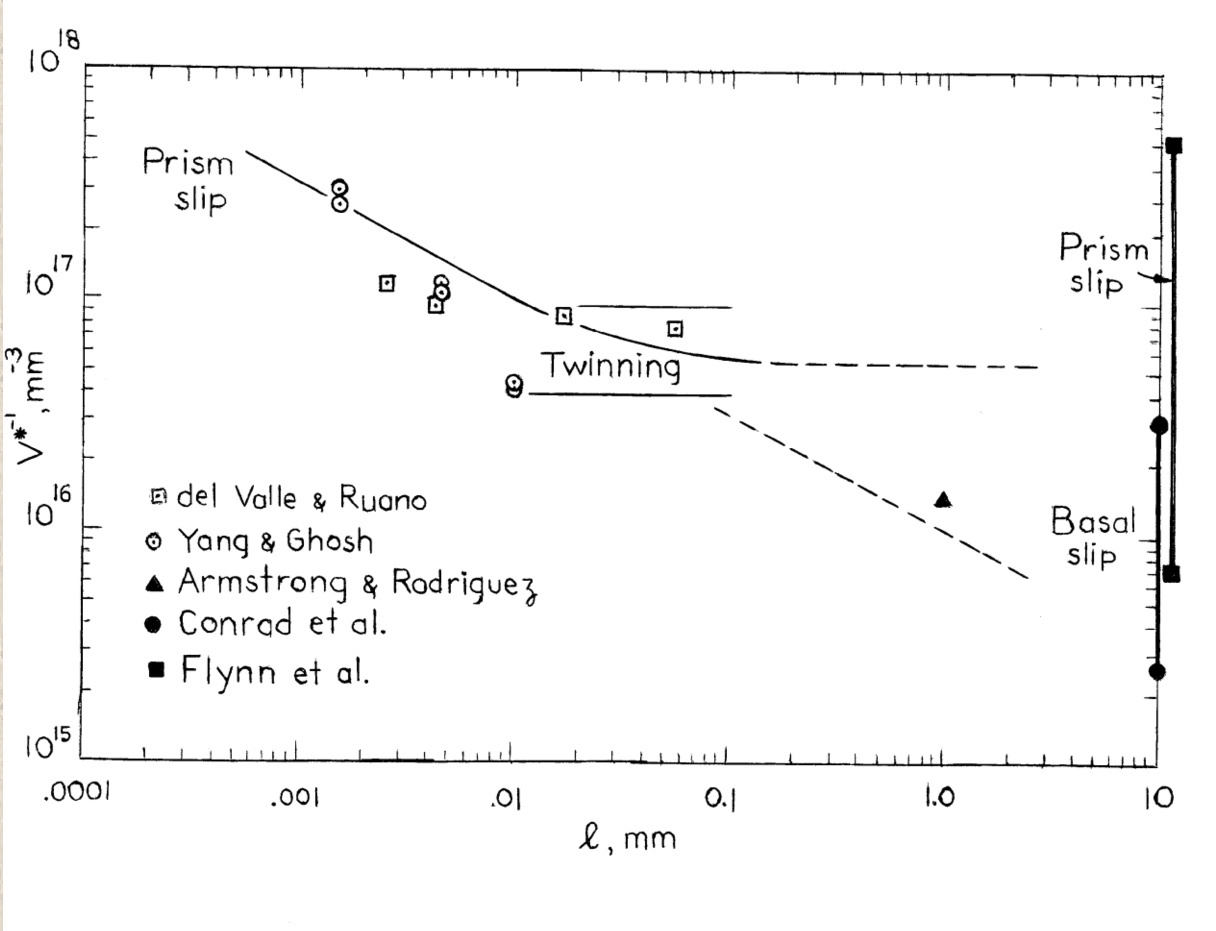
4. At small $\varepsilon$, $(\tau_{CTh} + \tau_G)v^*{}_C \sim \tau_{CTh}v^*{}_C \sim W_0$, and so an H-P type dependence is obtained for the polycrystal $v^{*-1}$

# An H-P type v*$^{-1}$ dependence for polycrystal Zn



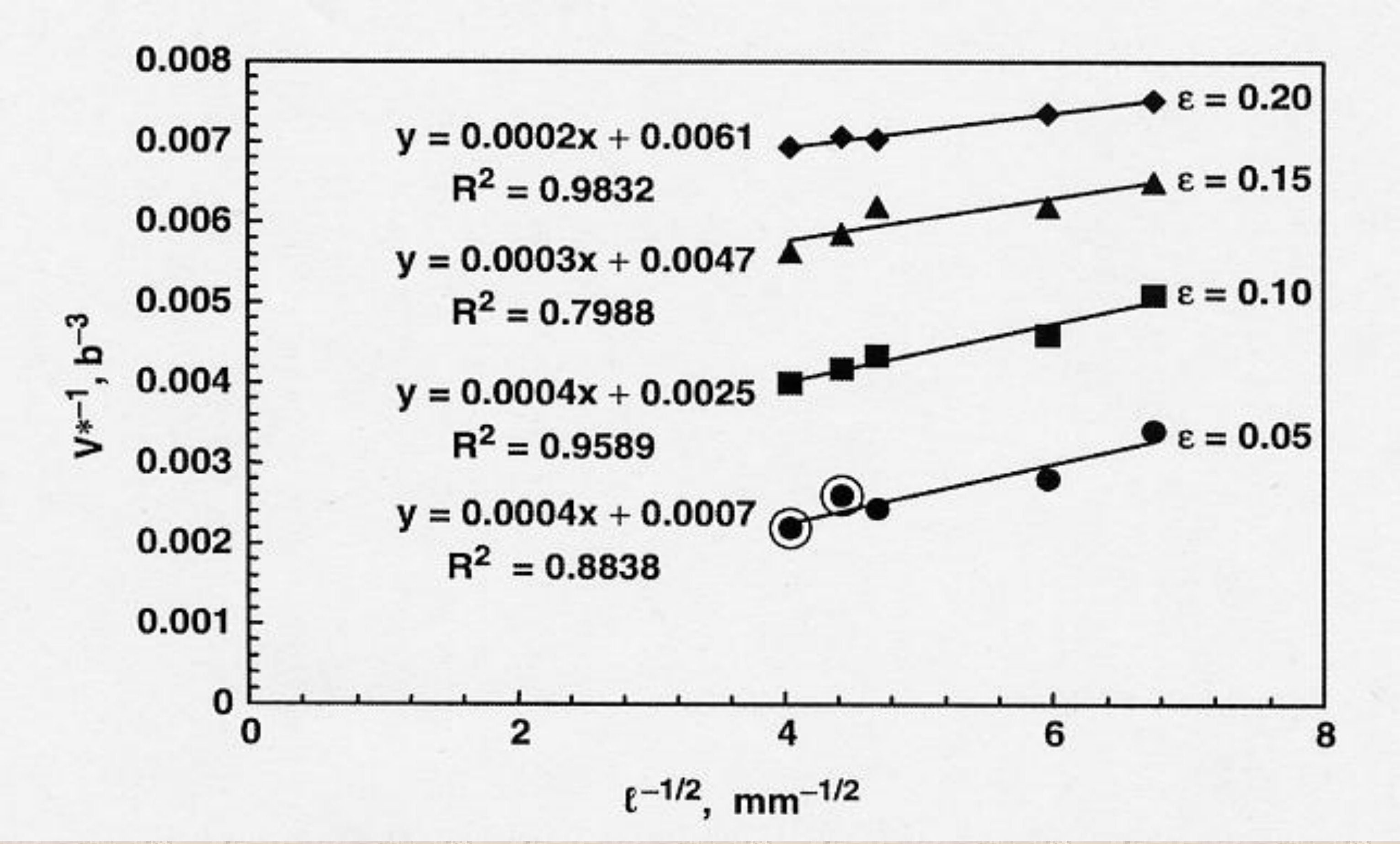

Y.V.R.K. Prasad *et al.*, in *Grain Boundaries in Engineering Materials; Fourth Bolton Landing Conference* (Claitor's Press, Baton Rouge, LA, 1974) pp. 529-536.

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



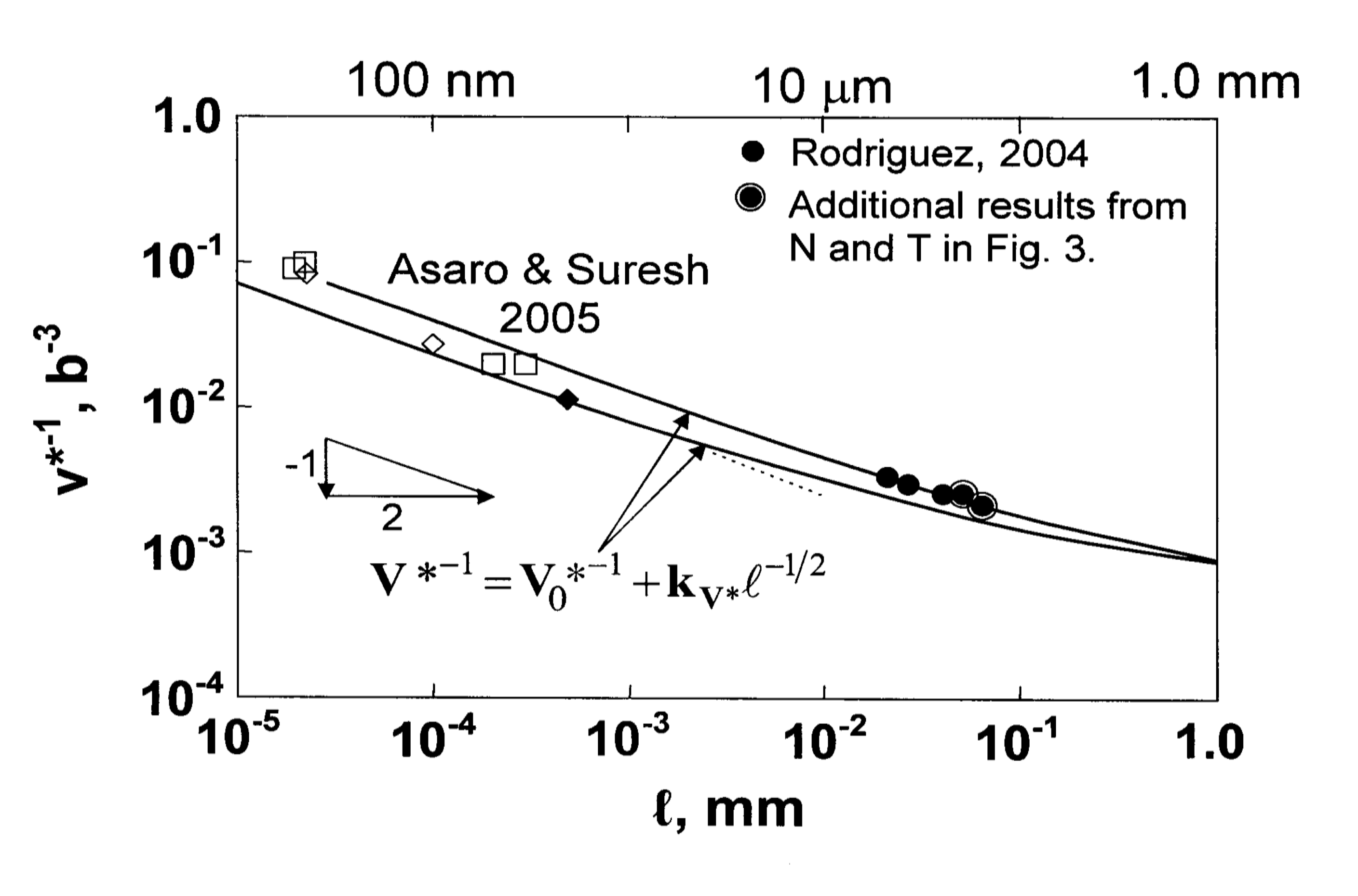

R.W. Armstrong, in *Mechanical Properties of Nanocrystalline Materials*, edited by J.C. M. Li (Pan Stanford Publ. Ltd., Singapore, 2011) Chap. 3, pp. 31-61

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



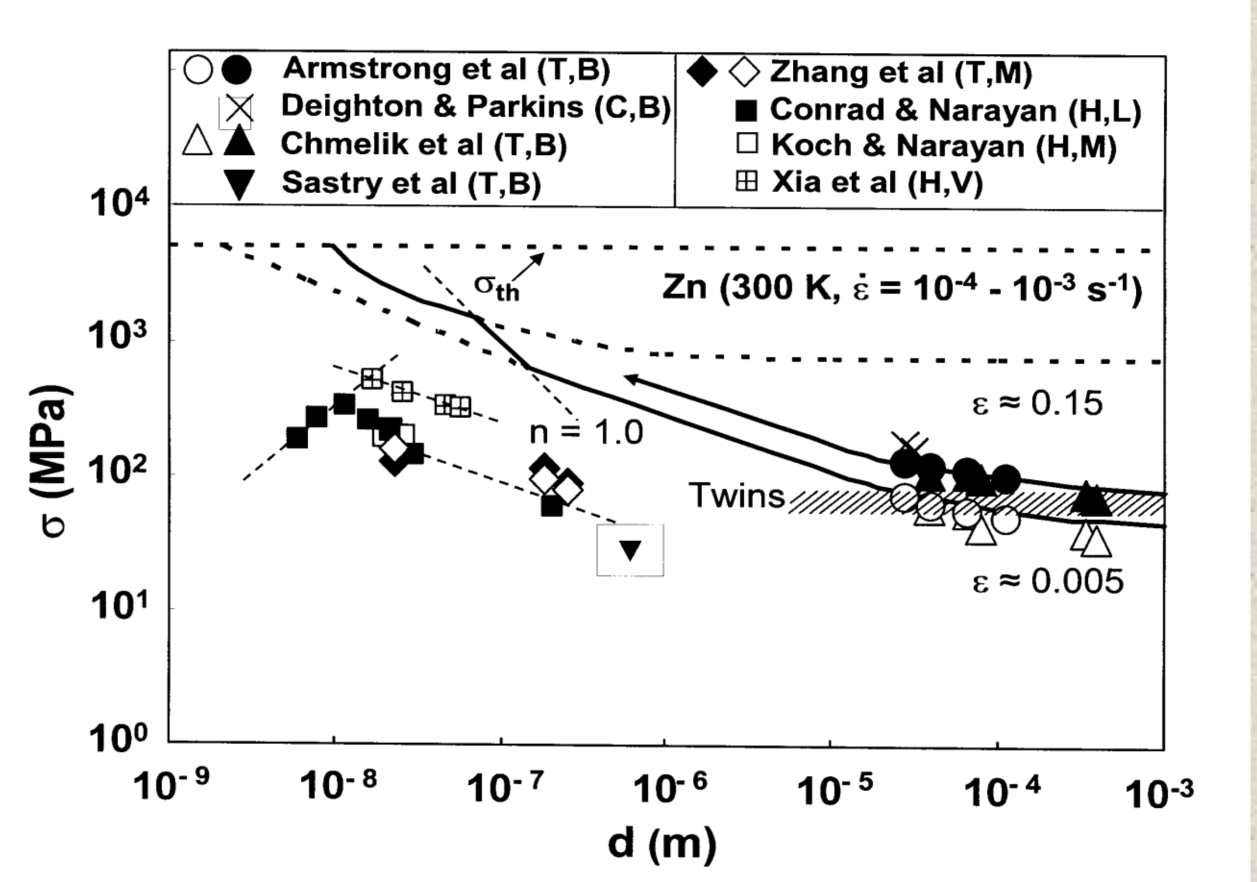

R.W. Armstrong and P. Rodriguez, *Philos. Mag.*, **86**, 5787-5796 (2006);
after T. Narutani and J. Takamura, *Acta Metall. Mater.*, **39**, 2037- 2049 (1991)

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



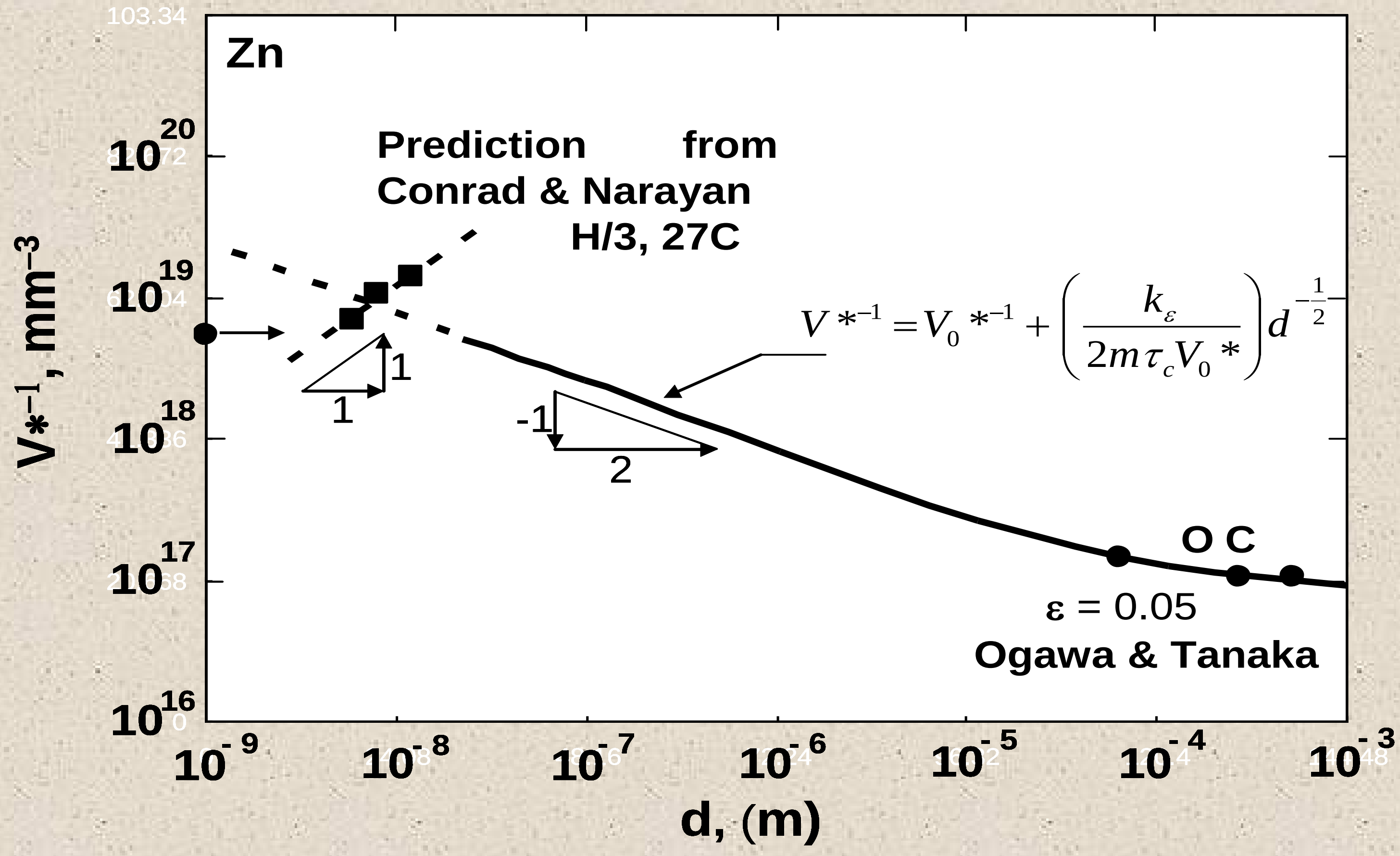

R.W. Armstrong and P. Rodriguez, *Philos. Mag.*, **86**, 5787-5796 (2006), after R.J. Asaro and S. Suresh, *Acta Mater.*, **53**, 3369-3382 (2005)

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



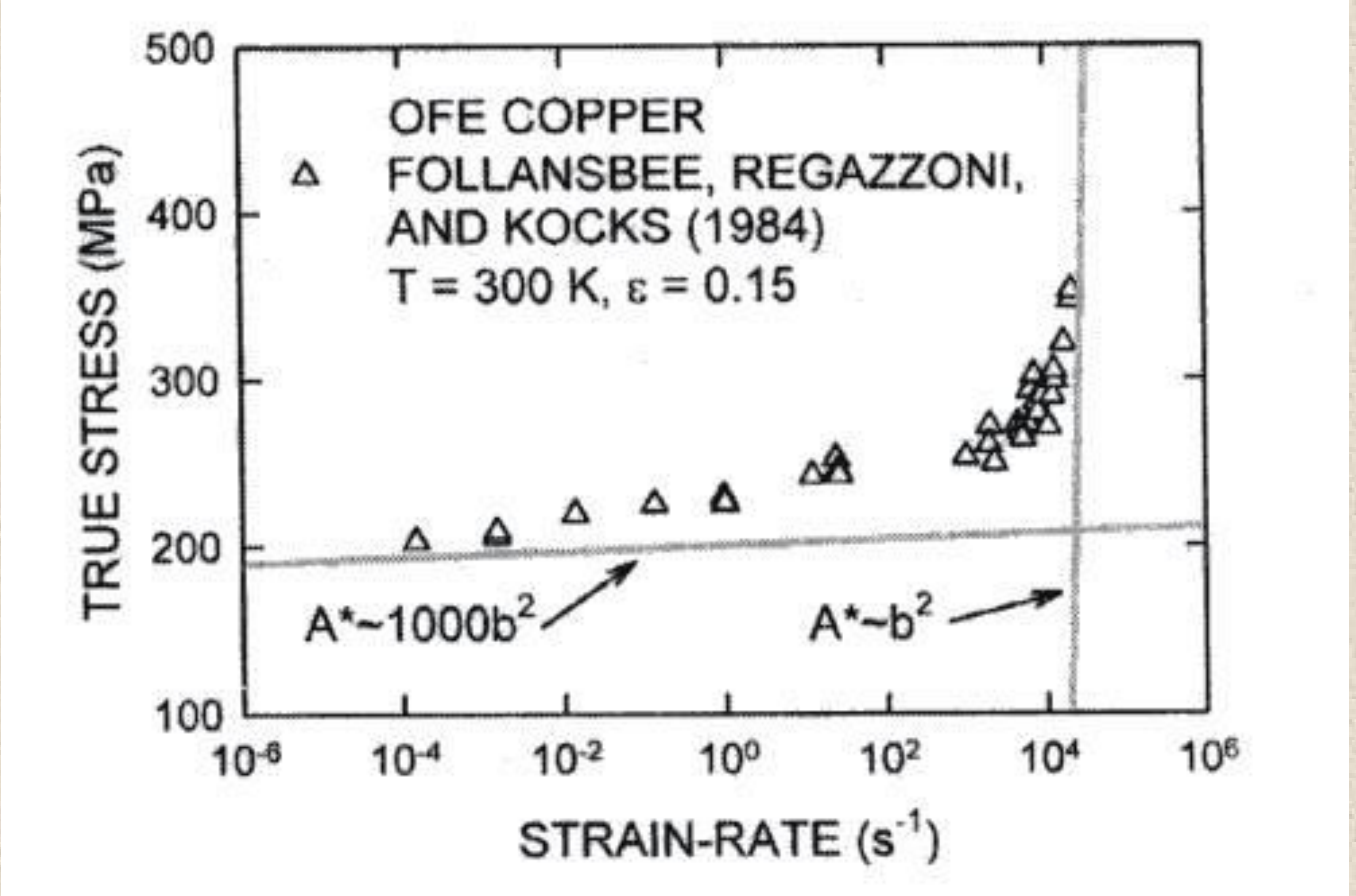

P. Rodriguez and R.W. Armstrong, *(Indian) Bull. Mater. Sci.*, **29**, 717-710 (2006); after H. Conrad and J. Narayan, *Acta Mater.*, **50**, 5067-5073 (2002)

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



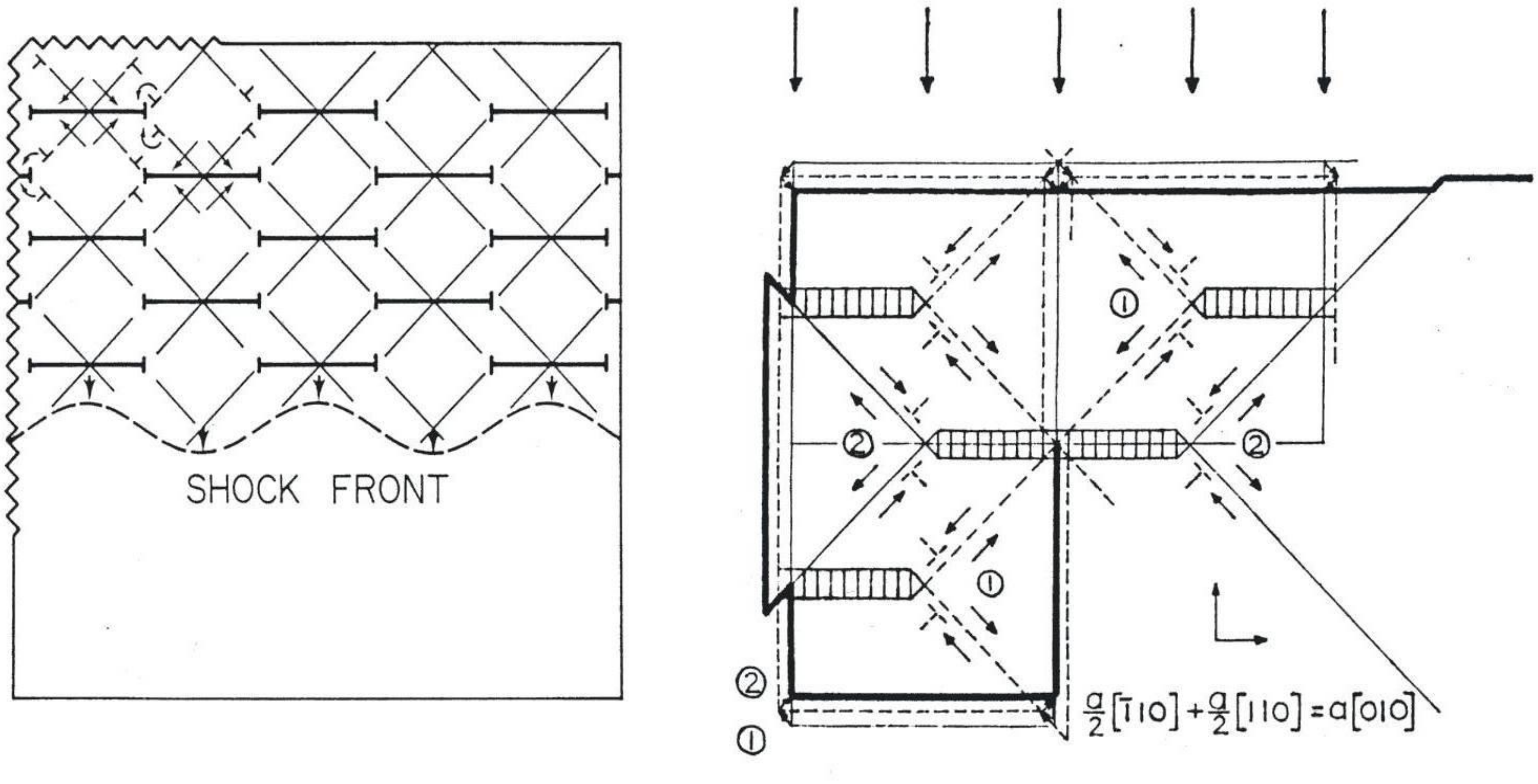

R.W. Armstrong, in *Mechanical Properties of Nanocrystalline Materials*, edited by J.C.M. Li (Pan Stanford Publ. Ltd., Singapore, 2011) Chap. 3, pp. 61-91.

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




R.W. Armstrong, W. Arnold, and F.J. Zerilli, *Metall. Mater. Trans. A*, **38A**, 2605-2610 (2007)

# Nanoscale dislocation generation at a propagating shock front

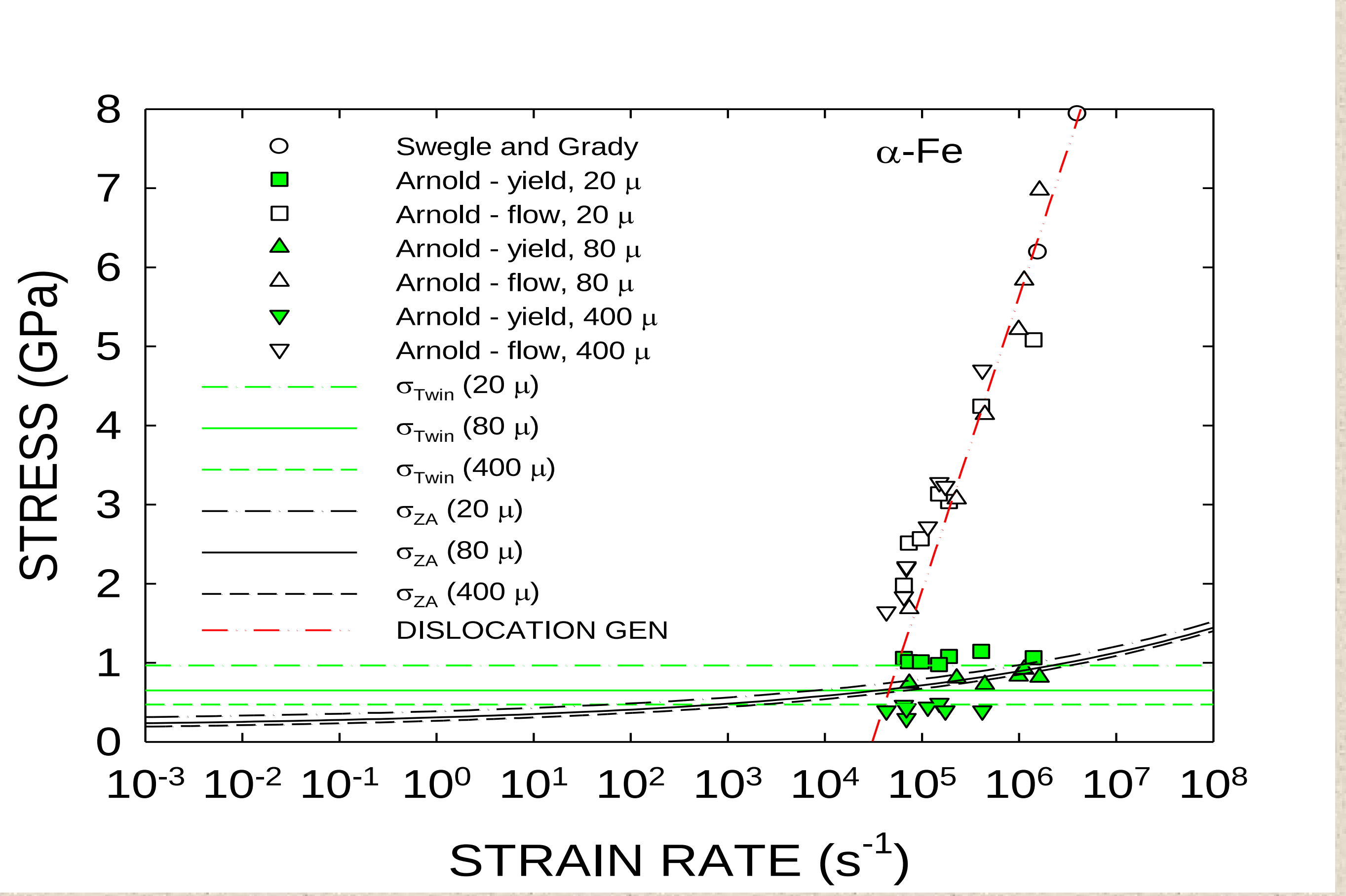



REACTED DIPOLES FROM SHEAR AT THE SHOCK FRONT

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

R.W. Armstrong, W. Werner, and F.J. Zerilli, *Metall. Mater. Trans. A*, **38A**, 2605-2610 (2007)

# Shocked Armco iron at different grain sizes and strain rates




## Plastic front propagation by nanoscale twinning

R.W. Armstrong, W. Arnold and F.J. Zerilli, *J. Appl. Phys.*, **105**, 023511 (2009)

# Shockless isentropic compression experiments (ICEs)

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

$$\sigma_{Th} = \{1 - [c(d\varepsilon/dt)/\beta_1 \sigma_{Th}]^{-\beta 1T}\}[B\mathbf{exp}(-\beta T)]$$

in which

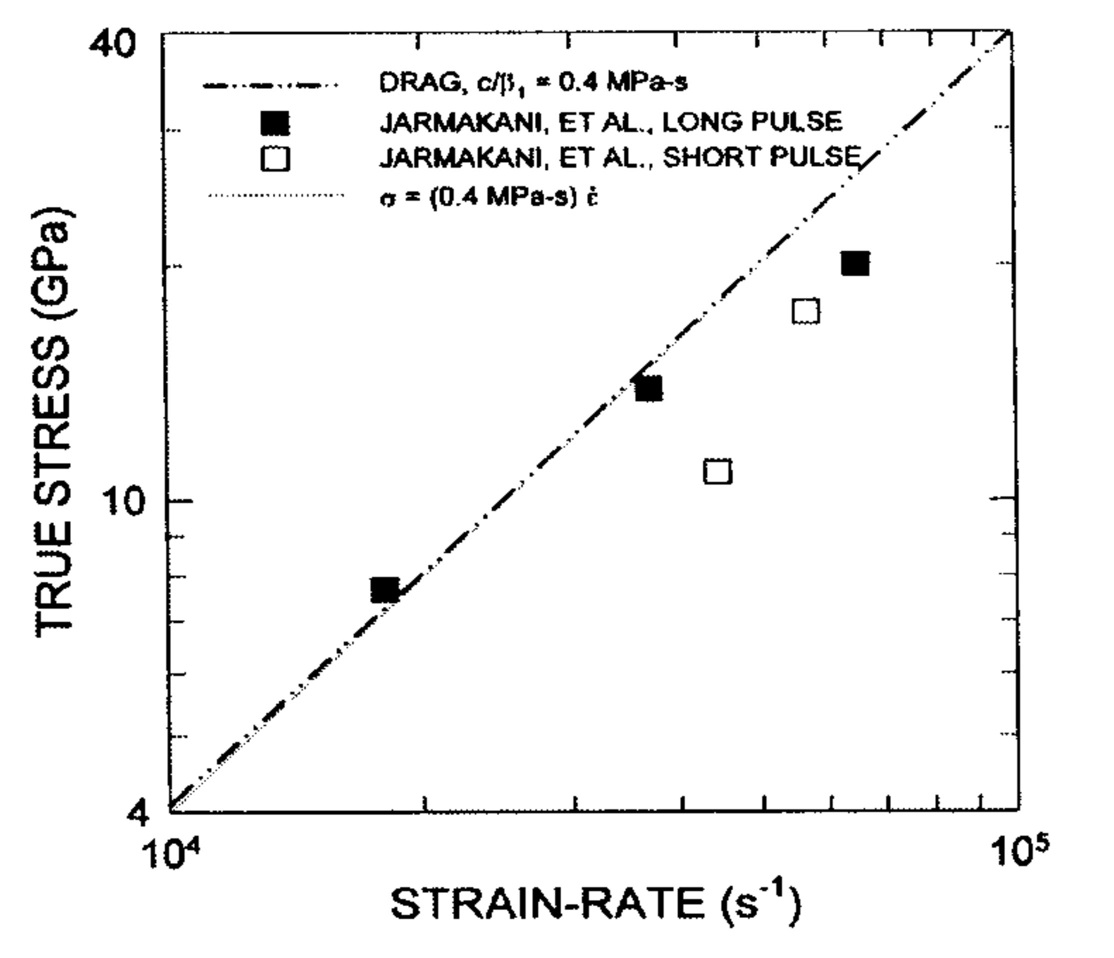
$$c = c_0 m^2 \beta_1/\rho b^2 \quad \text{and} \quad b\tau_{TH} = c_0 v.$$

At high $(d\varepsilon/dt)$:

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

F.J. Zerilli and R.W. Armstrong, *Acta Mater.*, **40**, 1803-1808 (1992);
R.W. Armstrong, W. Arnold and F.J. Zerilli, *J. Appl. Phys.* 105, 023511 (2009)

# Drag-controlled shockless ICE results for copper




R.W. Armstrong, W. Arnold and F.J. Zerilli, *J. Appl. Phys.*, **105**, 023511 (2009)

# 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.