MULTISCALE GRAIN SIZE AND VISCOPLASTICITY ASPECTS OF (NANO)POLYCRYSTAL DEFORMATION BEHAVIORS*

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TOPICS

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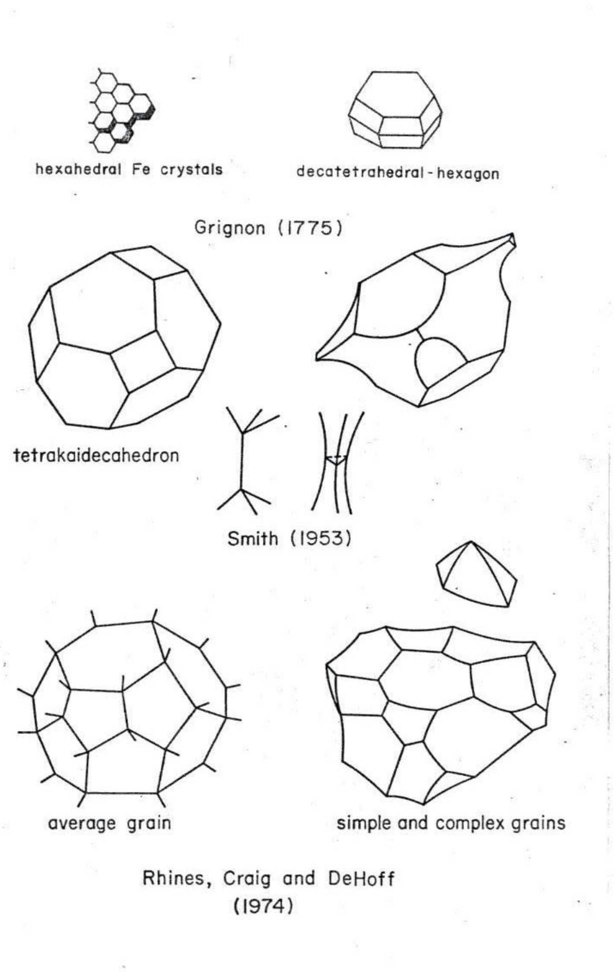
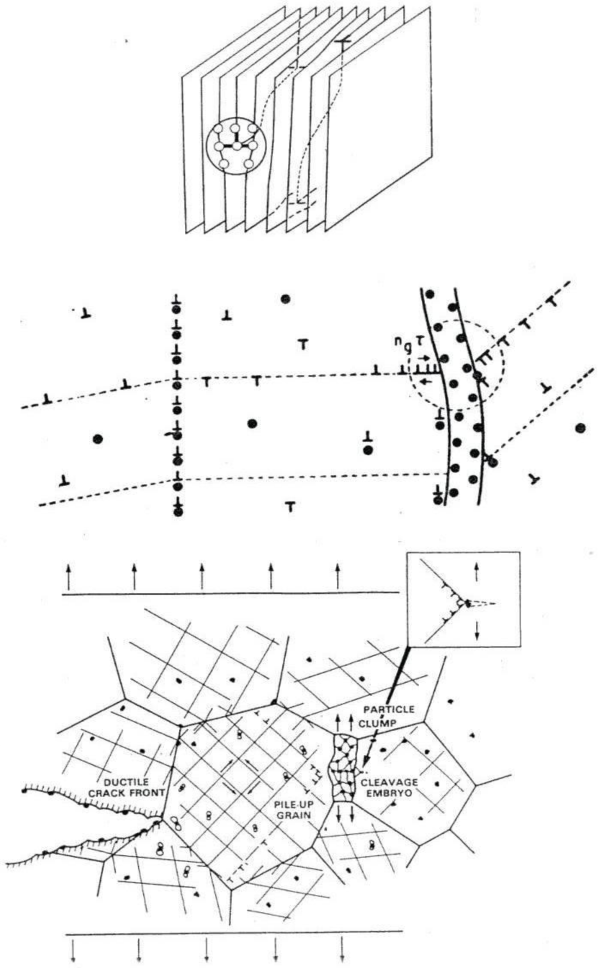
Polycrystals and Dislocations





Constitutive Equations and Parameters

The total range for creep, slip, twinning and cleavage dynamics:
$\varepsilon = \gamma/m$; $\varepsilon = \varepsilon\{\Delta t, \sigma, D, T\} \rightarrow \sigma = \sigma\{(d\varepsilon/dt), T, \ell^{-1/2}\}$; $\sigma = m\tau$
$2.0 \leq m \leq 3.1$ for fcc structures; $(d\sigma/d\varepsilon) = m^2(d\tau/d\gamma)$

1. Thermal activation-strain rate analysis: $(d\varepsilon/dt) = (d\varepsilon/dt)\{T, \tau_{Th}\}$;
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 $(d\varepsilon/dt) = (d\varepsilon/dt)_0\mathbf{exp}\{-(G_0 - \int v^* d\tau_{Th})/kT\}$, 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 equation and microstructural stress intensities, k_ε'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 $\sigma = m[(\tau_G + \tau_{Th}) + (\pi m^* Gb\tau_C/2\alpha)^{1/2}\ell^{-1/2}] = \sigma_{0\varepsilon} + k_\varepsilon\ell^{-1/2}$
and $k_{Al} < k_{Cu} < k_{Mg} << k_{\alpha\text{-}Fe}$ with $k_\varepsilon < k_{y.p.} << k_T \sim k_C << K_{IC}$
with c and ℓ analogous in comparison with the fracture mechanics pre-crack plane strain stress intensity expressed as $K_{Ic} = \sigma(\pi c)^{1/2}$

3. Shock $[(d\rho/dt)b\Delta x]$ vs. ICE $[\rho b\upsilon']$ for $(d\gamma/dt)$.

Thermal Activation – Strain Rate Analysis (TASRA)

$$d\gamma/dt = {}_{i}\sum^{N} b_{i}(d[\Delta A]_{i}/dt)/AL = \rho b[dx/dt]$$

$$d\gamma/dt = \rho b(dx/dt)_{0}\mathbf{exp}\{(-\Delta G_{0} + \int bA^{*}d\tau^{*})/k_{B}T\}$$

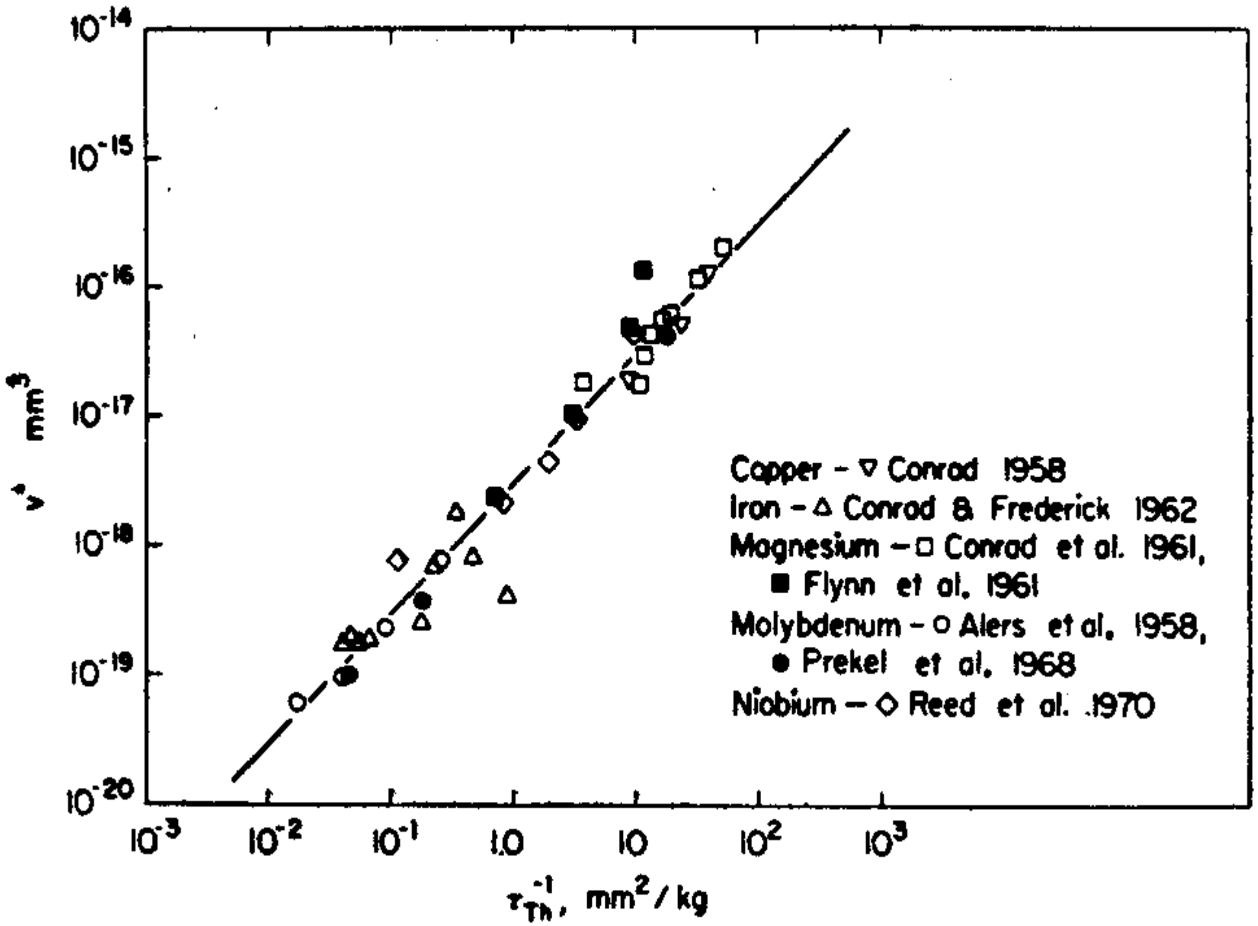
$$v^{*} \equiv bA^{*} \equiv k_{B}T[\partial \mathbf{ln}(d\gamma/dt)/\partial\tau^{*}]_{T} = W_{0}/\tau^{*}$$

References:

1. E. Orowan, Proceedings of the Physical Society, London, B52, 8-22 (1940)
2. G. Schoeck, Physica Status Solidi, 8, 499-507 (1965)
3. R.W. Armstrong, (Indian) J. Sci. & Indust. Res., 32, 591-598 (1973)

Experimental v* Measurements

Reference: R.W. Armstrong, (Indian) J. Sci. & Indust. Res., 32, 591-598 (1973); F.J. Zerilli and R.W. Armstrong, J. Appl. Phys., 61, 1816-1825 (1987); R.W. Armstrong and S.M. Walley, Intern. Mater. Rev., 53, [3], 105-128 (2008)



Polycrystal Hall-Petch (H-P) Dislocation Pile-up Analysis

$$\sigma_\varepsilon = m\tau_{0\varepsilon} + mk_{S\varepsilon}\ell^{-1/2};\ m\tau_0 = \sigma_0,\ mk_{S\varepsilon} = k_\varepsilon$$

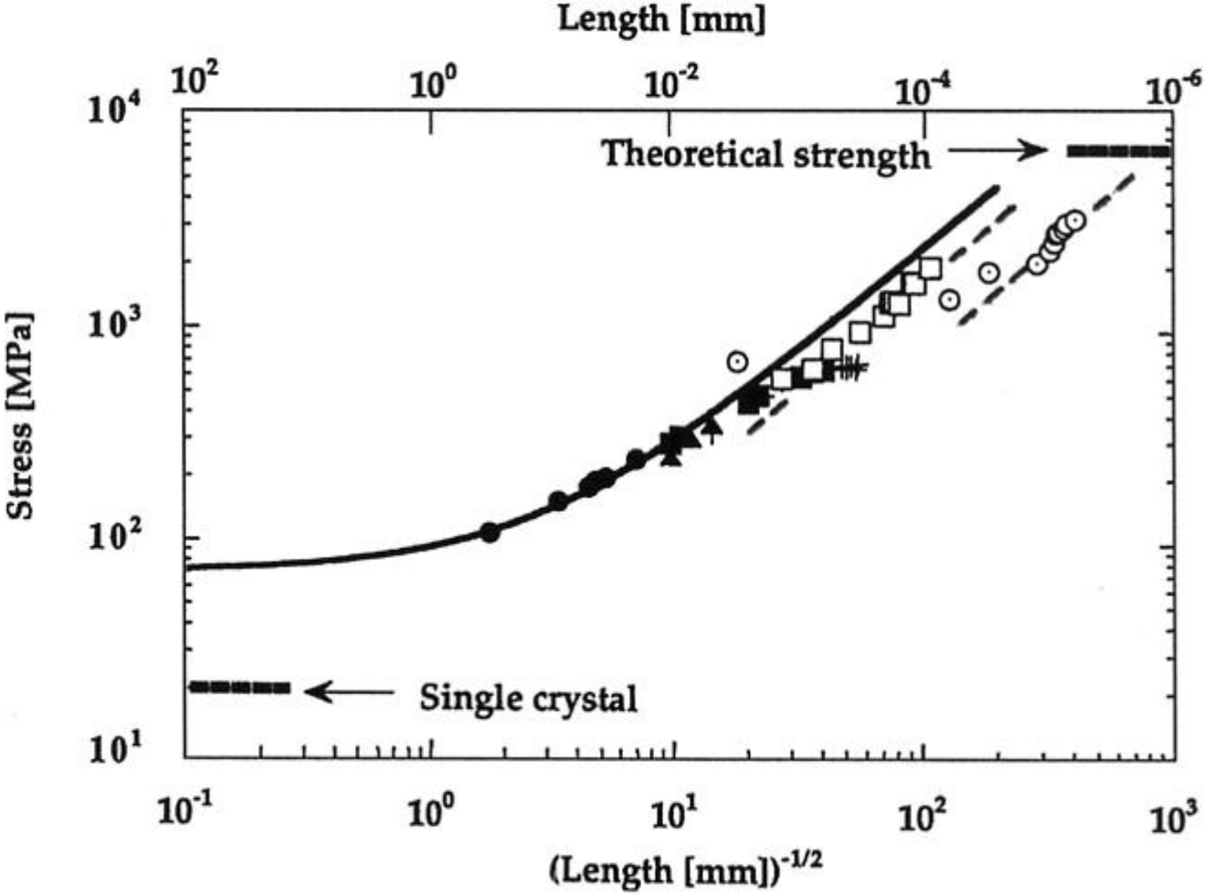
$$\sigma_{0\varepsilon} = m[\tau_{0\varepsilon G} + \tau_{0\varepsilon}{}^*]$$

$$k_\varepsilon = m[\pi m^* G b \tau_C/2\alpha]^{1/2}$$

References:

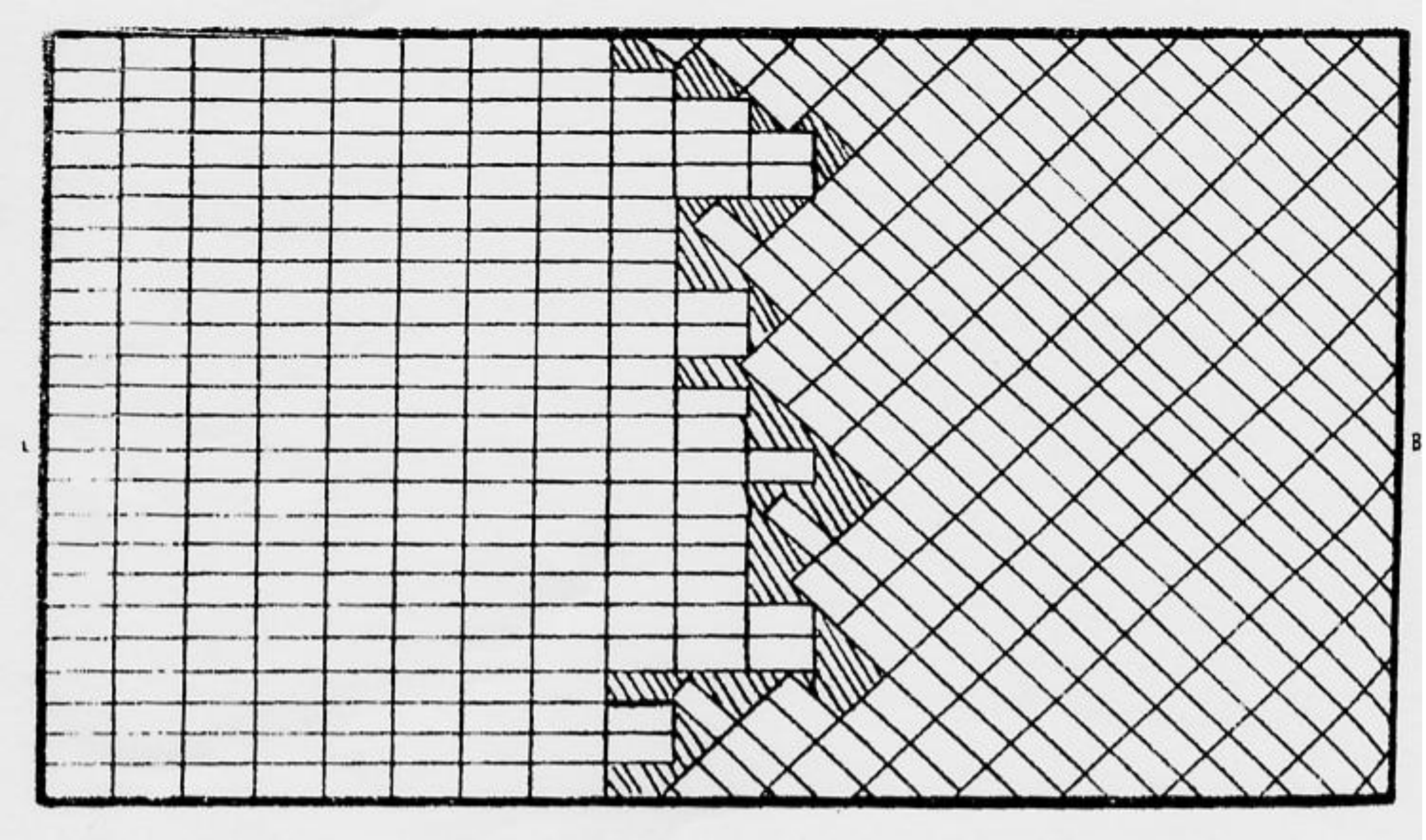
1. R.W. Armstrong, I. Codd, R.M. Douthwaite and N.J. Petch, Philosophical Magazine, 7, 45-53 (1962)
2. R.W. Armstrong, Acta Metallurgica, 16, 347-355 (1968)
3. R.W. Armstrong, “Yield, Flow and Fracture of Polycrystals” (ed. T.N. Baker) Applied Science Publishers, London, U.K., pp. 1-31 (1983)

Hall-Petch results for iron and steel



R.W. Armstrong, “*Grain boundary structural influences on nanopolycrystal strength and strain rate sensitivity*”, Special Issue of **Emerging Materials Research**, in honor of Professor J. Narayan 2011 Acta Materialia Gold Medal Award, 2012.

The history of grain boundary disorder



"…the portions shaded black in the diagram will remain in the amorphous condition. …"

Walter Rosenhain and Donald Ewen, "*Intercrystalline Cohesion in Metals*", *J. Inst. Met.*, **8**, 149-173 (1912)

H-P microstructural stress intensities, k_ε's

(1) $K_{Ic} >> k_C > k_T >> k_\varepsilon$ for **α-Fe** are

(>600) >> ~100 > ~90 >> ~24 $MPa.mm^{1/2}$

from pre-cracked fracturing to crack-free yielding

(2) For texture-free **Mg**,

k_ε = ~10 $MPa.mm^{1/2}$

for needed {10-10}<11-20> prism slip;

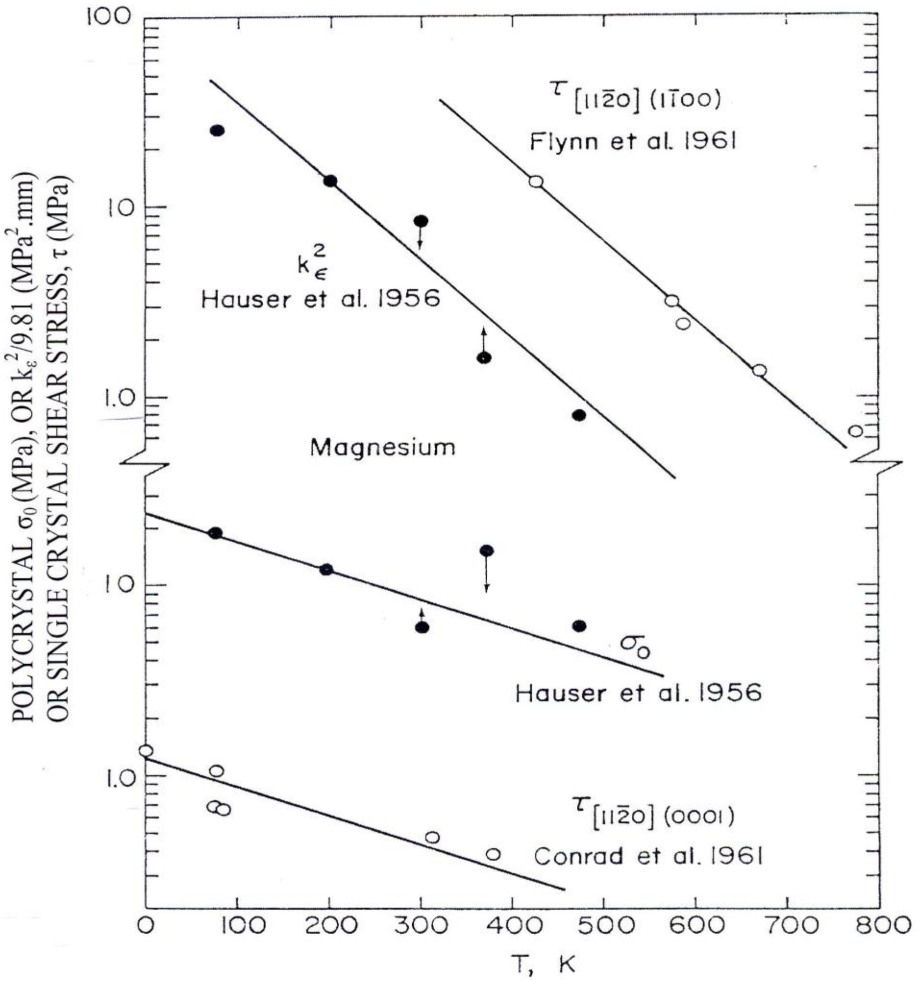
Zn and **Cd** needing pyramidal slip.

(3) For **Cu** and **Ni**, k_ε = ~5 $MPa.mm^{1/2}$,and

for **Al**, k_ε = ~1, in each case for cross-slip.

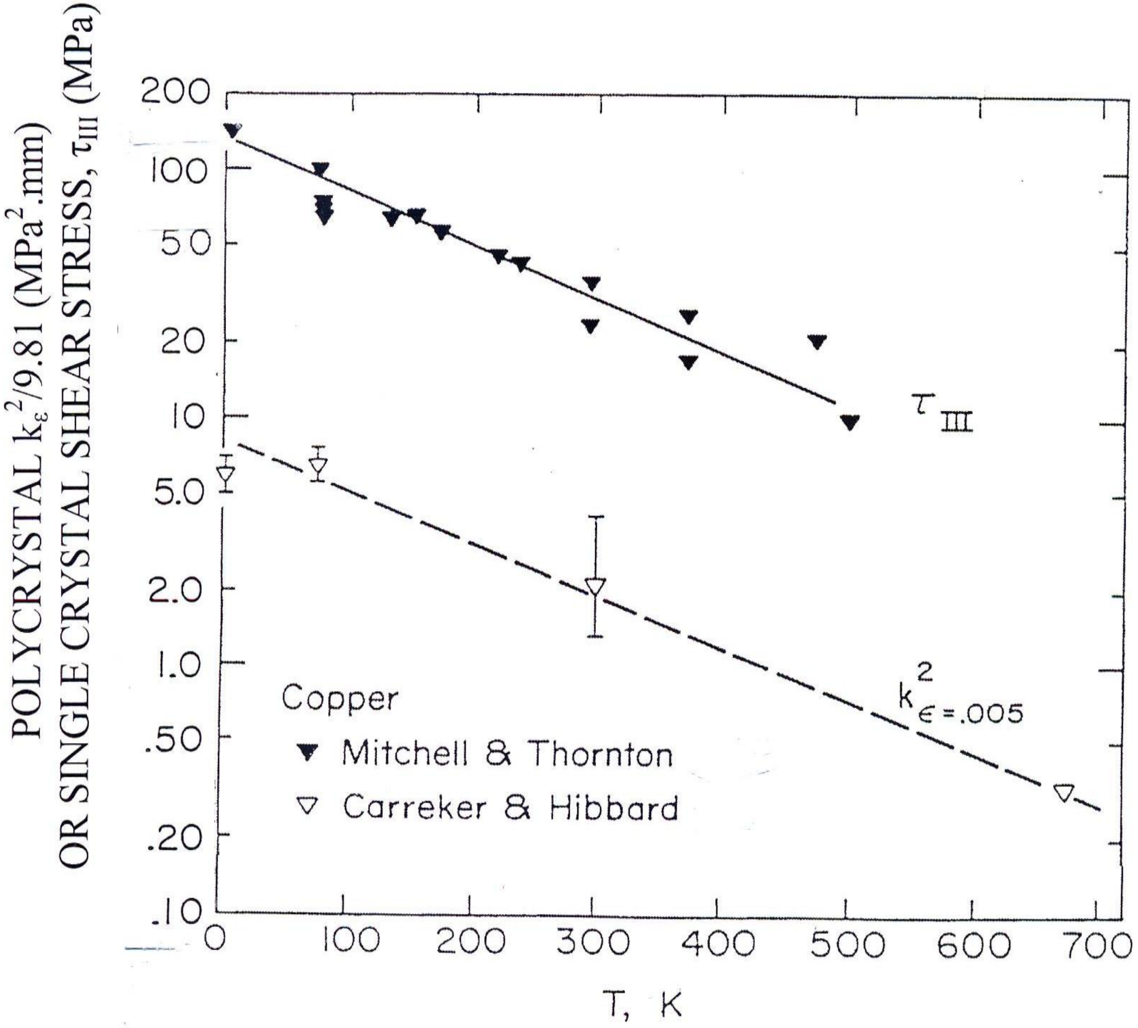
σ_0 , k_ε^2, and τ_{CRSS} Dependencies on T

Reference: R.W. Armstrong, Acta Metallurgica, 16, 347-355 (1968)



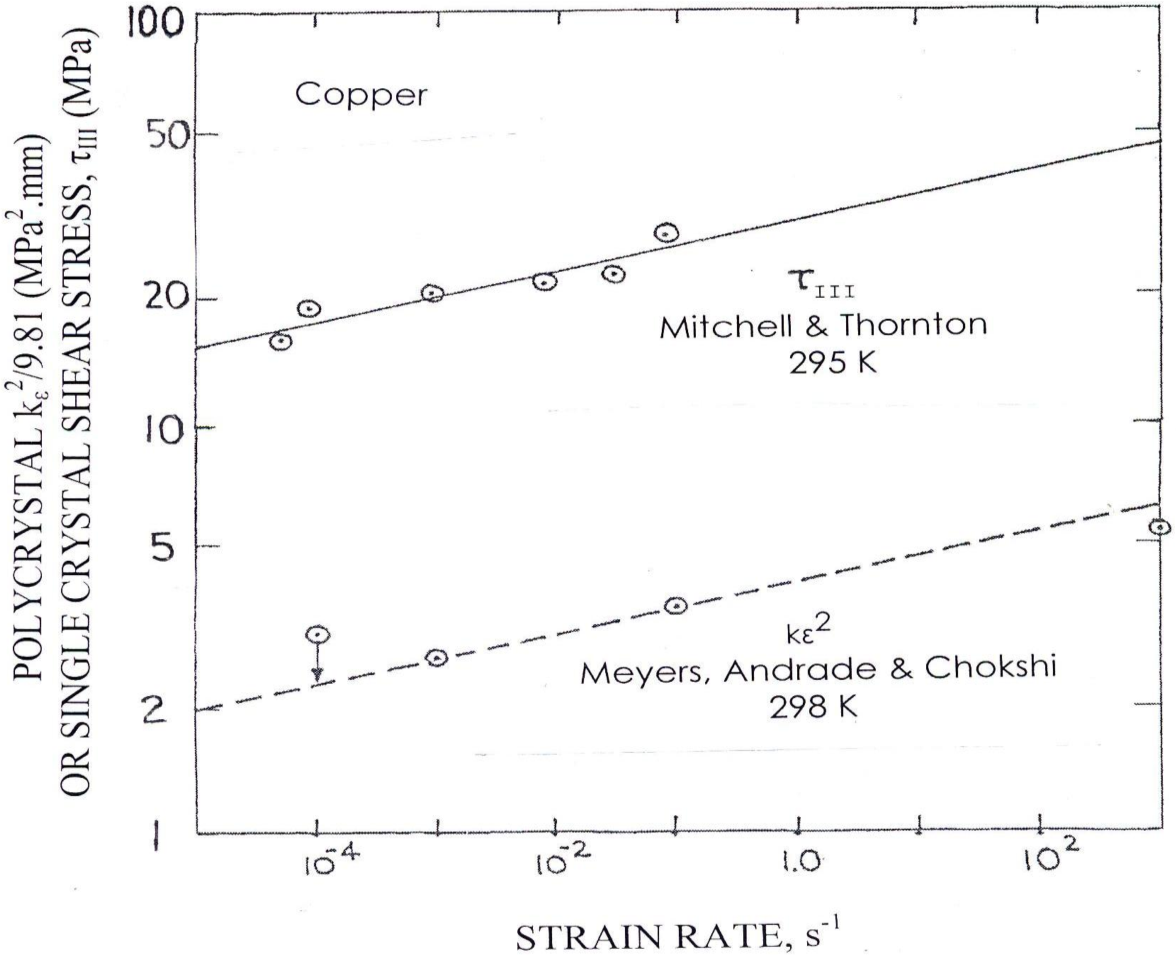
k_{ε}^{2} and Cross-Slip τ_{III} Dependence on T

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



k_{ε}^2 and τ_{III} Dependence on Strain Rate

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



v^{*-1} Measurement of Strain Rate Sensitivity

For a polycrystal, $v^{*-1} = (1/mkT)[\partial\sigma_{\varepsilon}/\partial\mathbf{ln}(d\varepsilon/dt)]_T$ but with TASRA dependence in both $\sigma_{0\varepsilon}$ and k_{ε}

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

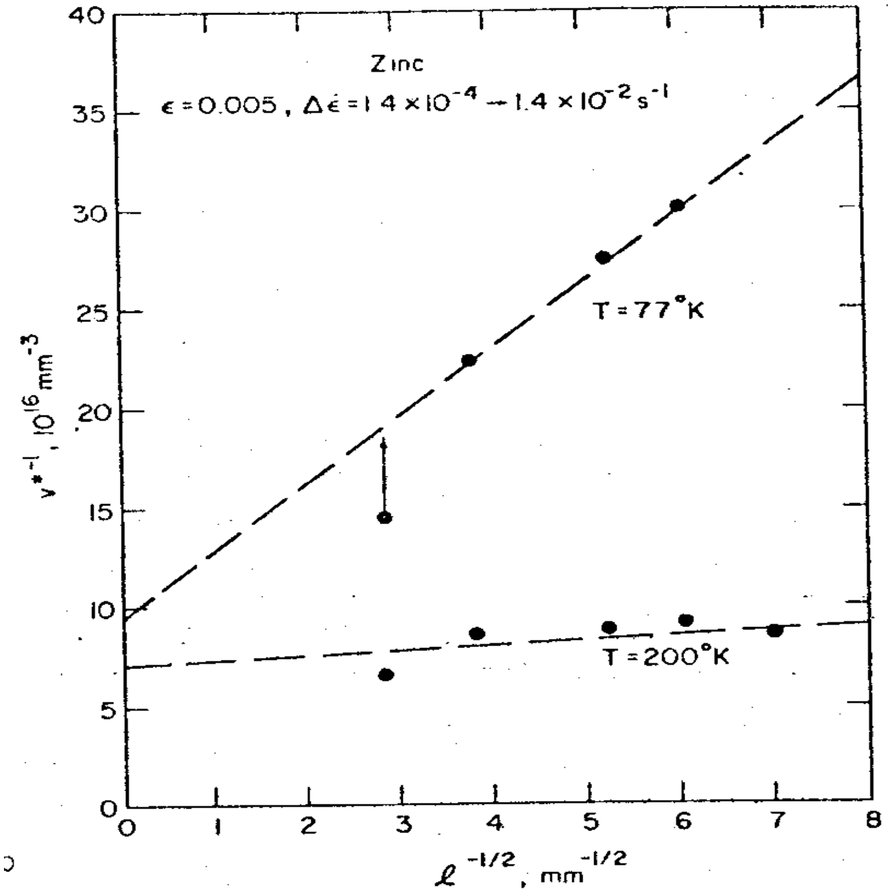
$$v^{*-1} = v_0{}^{*-1} + (k_{\varepsilon}/2m\tau_{C\varepsilon}v_C{}^{*})\ell^{-1/2}$$

References:

1. Y.V.R.K. Prasad and R.W. Armstrong, Philos. Mag., 29, 1421-1425 (1974)
2. P. Rodriguez, R.W. Armstrong, and S.L. Mannan, Trans. Indian Inst. Met., 56, 189-196 (2003)

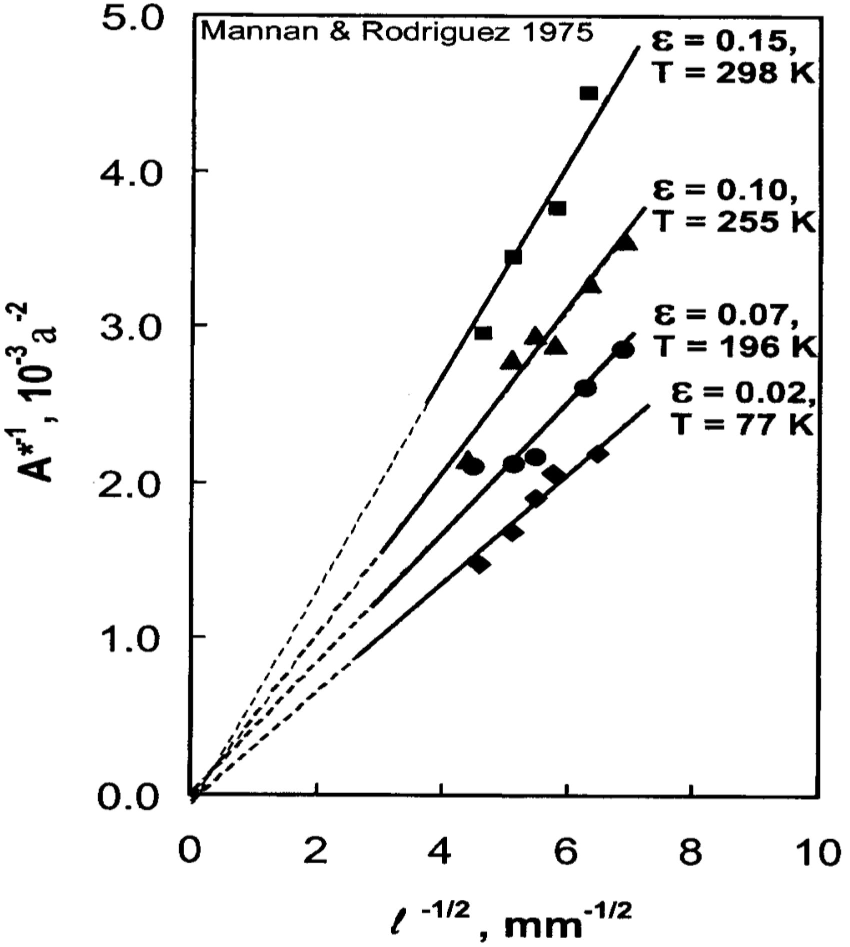
A Hall-Petch-Type Dependence for v^{*-1}

Reference: Y.V.R.K. Prasad, N.M. Madhava and R.W. Armstrong, “Grain Boundaries in Engineering Materials”, Fourth Bolton Landing Conference, N.Y., 1974 (Claitor’s Press, Baton Rouge, LA, 1975) pp. 67-75**.**



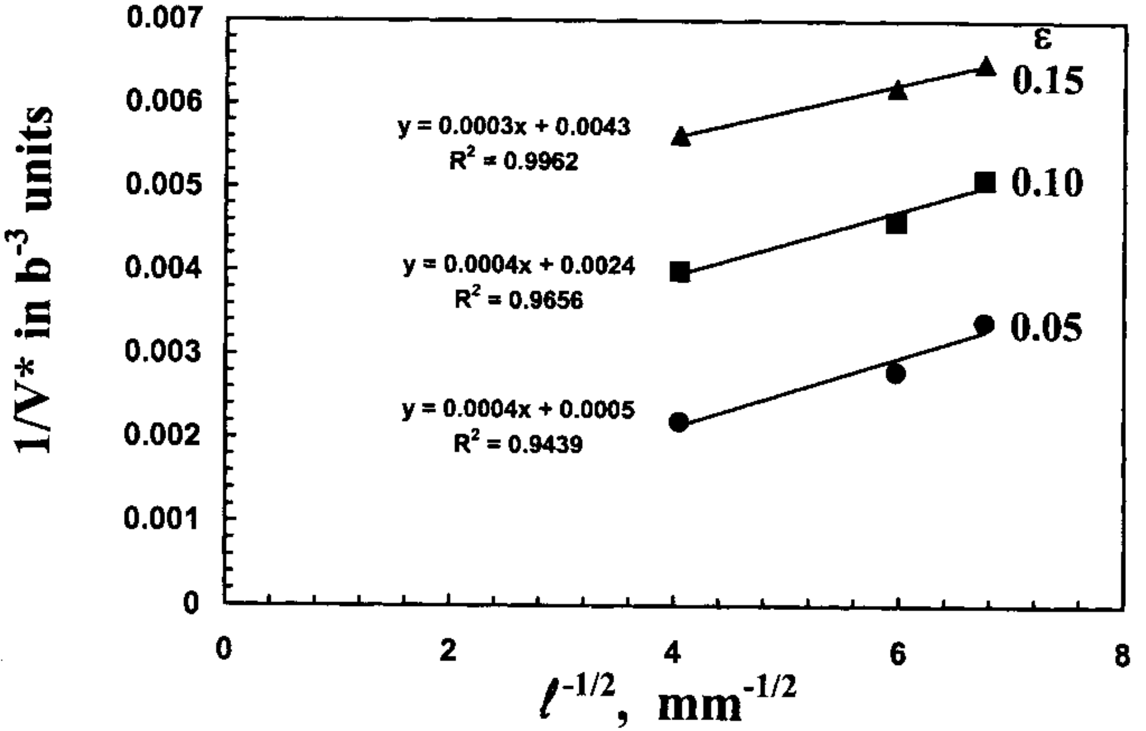
A Hall-Petch-Type Dependence of A^{*-1} Measurements for Cd

Reference: P. Rodriguez, Metall. Mater. Trans. A, 35A, 2697-2705 (2004)



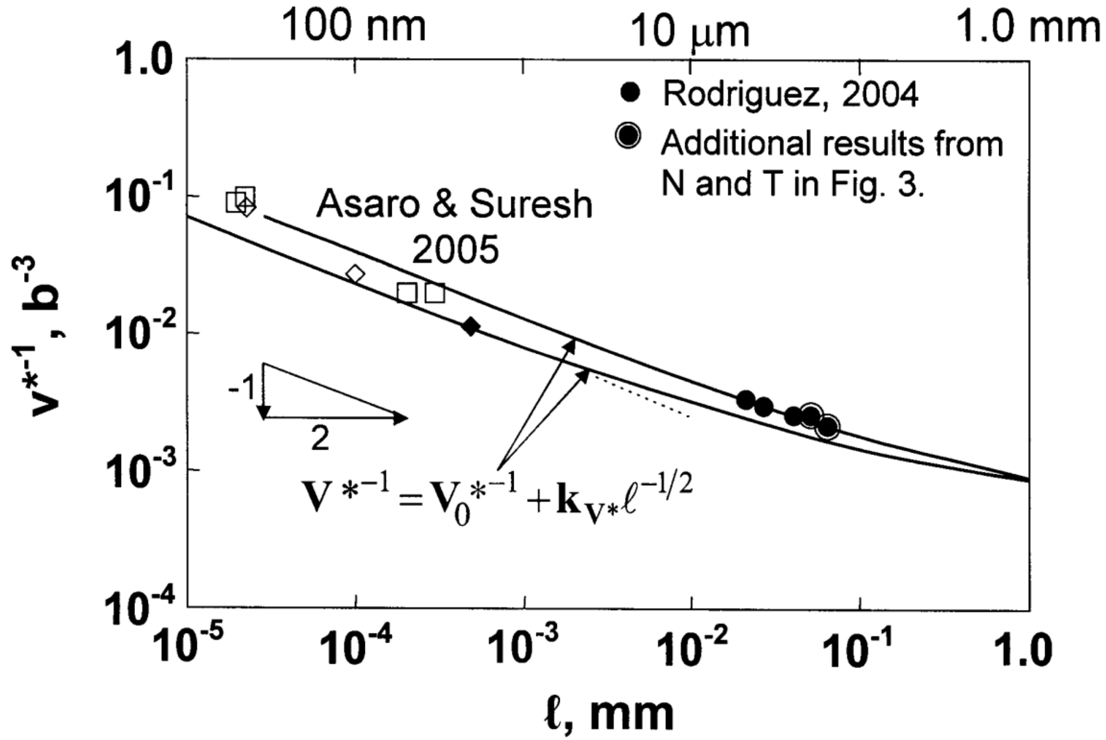
Hall-Petch-Type v^{*-1} for Ni Involving v_0^{*-1} (for Dislocation Intersections) Plus $\ell^{-1/2}$ Dependence (for Cross-Slip)

Reference: P. Rodriguez, Metall. Mater. Trans. A, 35A, 2697-2705 (2004); and, T. Narutani and J. Takamura, Acta Metall. Mater. 39, 2037-2049 (1991)



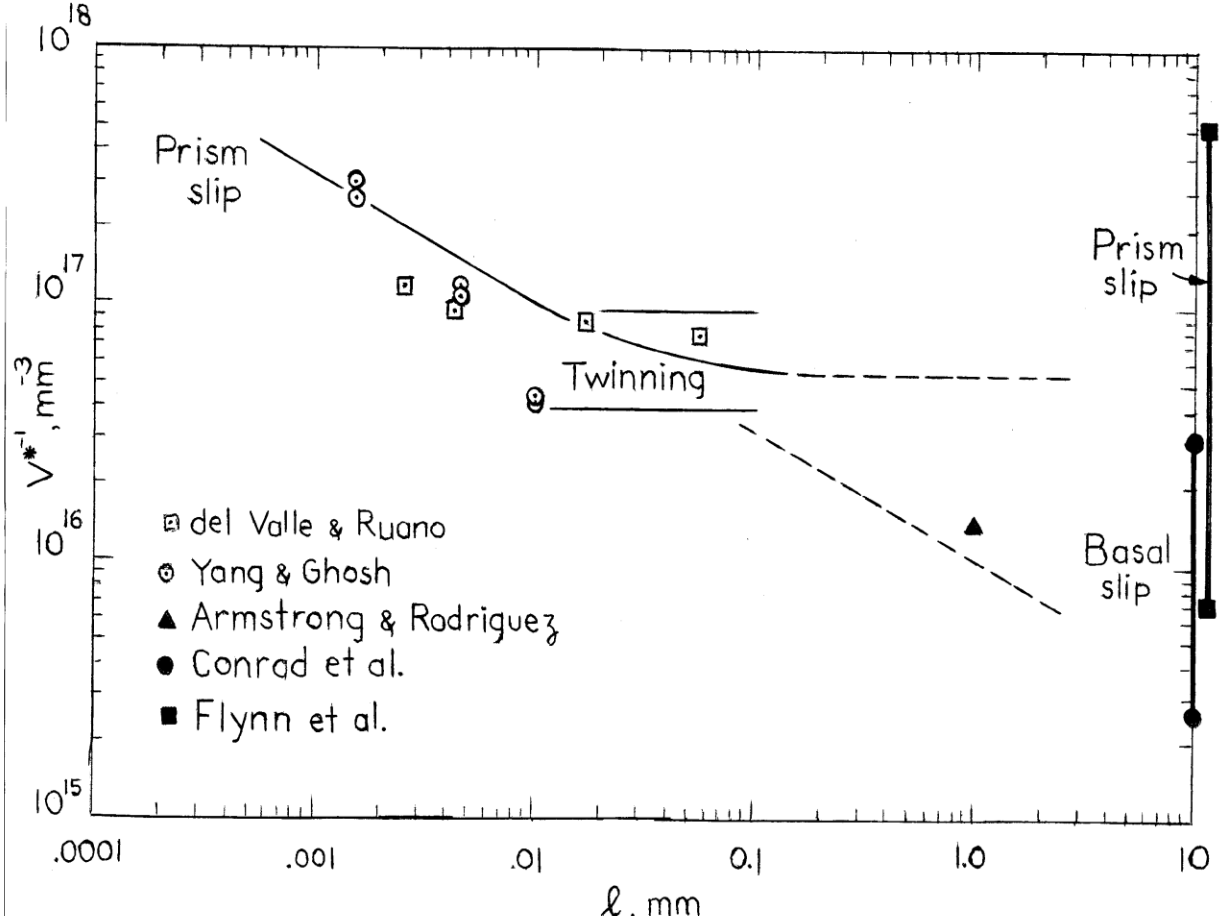
Conventional and Nanopolycrystal Hall-Petch Dependence for Compiled Cu and Ni Measurements of v*

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



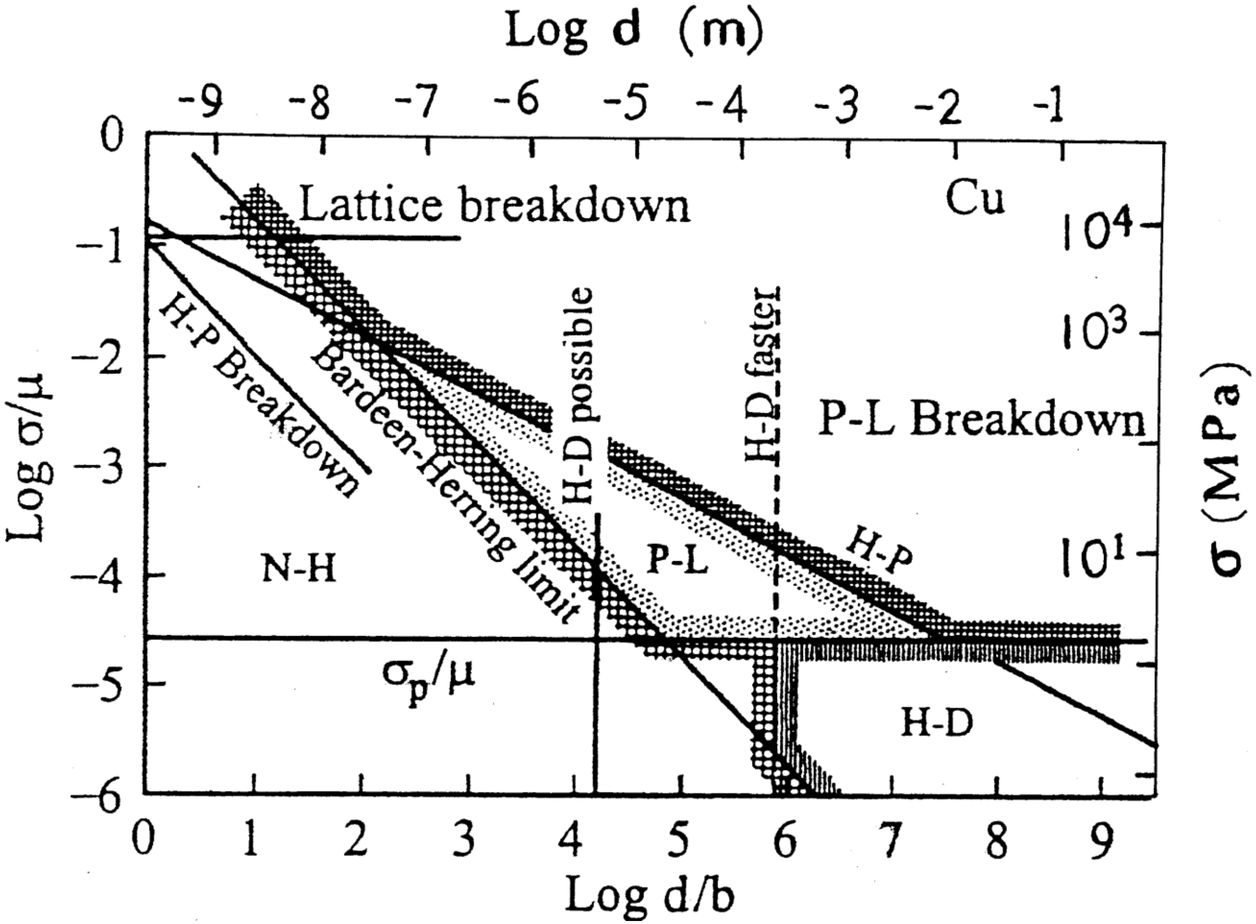
Hall-Petch-type v^{*-1} Dependence for Mg Spanning Single Crystal and Polycrystal, Basal and Prism, Slip Measurements

Ref.: P. Rodriguez, S. Venugopal, and R.W. Armstrong, unpublished (2008)



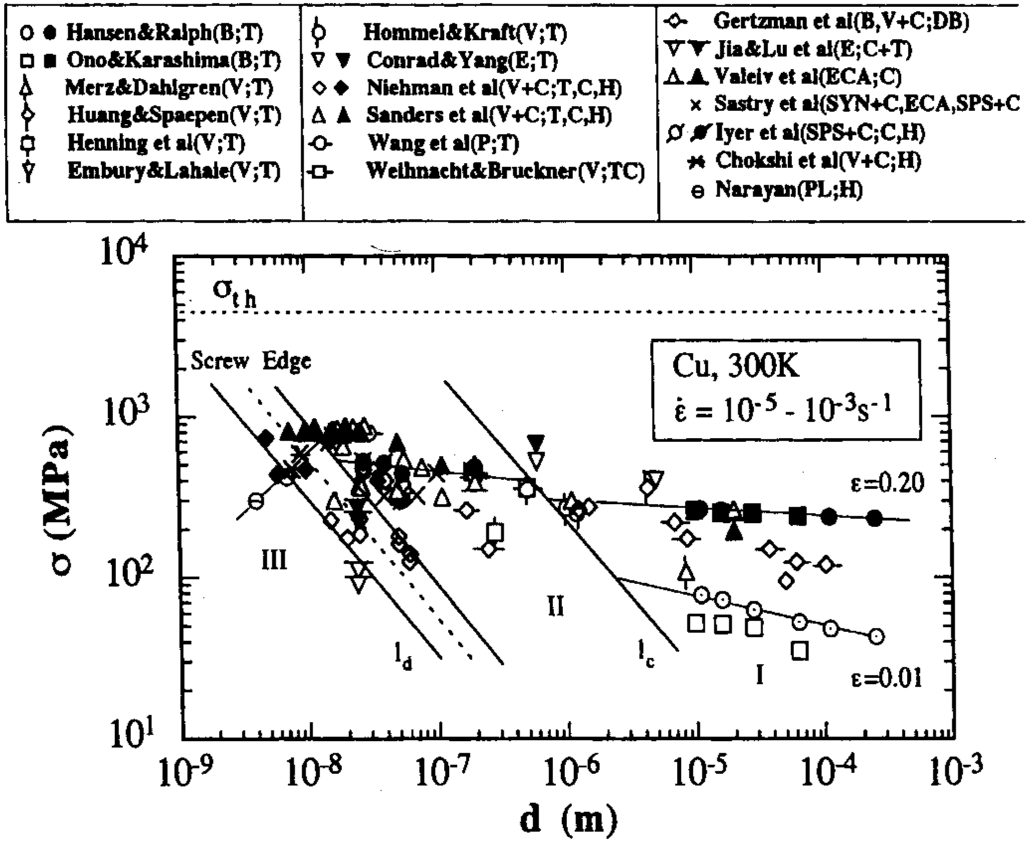
Nanopolycrystal Strength Dependence on Grain Size via a Limiting Creep Rate Model

Reference: F.R.N. Nabarro, Soviet Phys. – Solid State Phys., 42, 1417ff (2000)



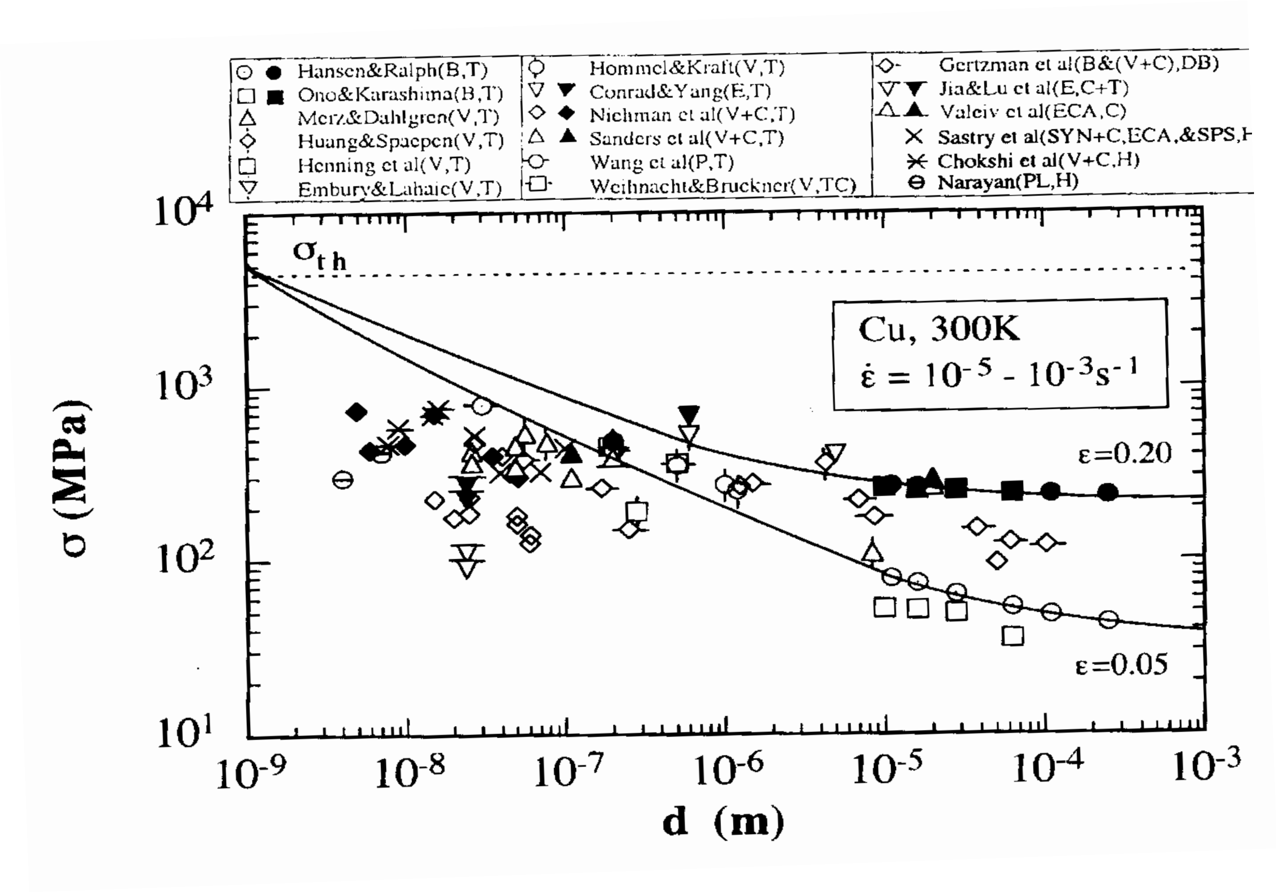
Compilation and Analysis of Conventional and Nanopolycrystal Strength Measurements

Reference: H. Conrad, Metall. Mater. Trans. A, 35A, 2681-2695 (2004)



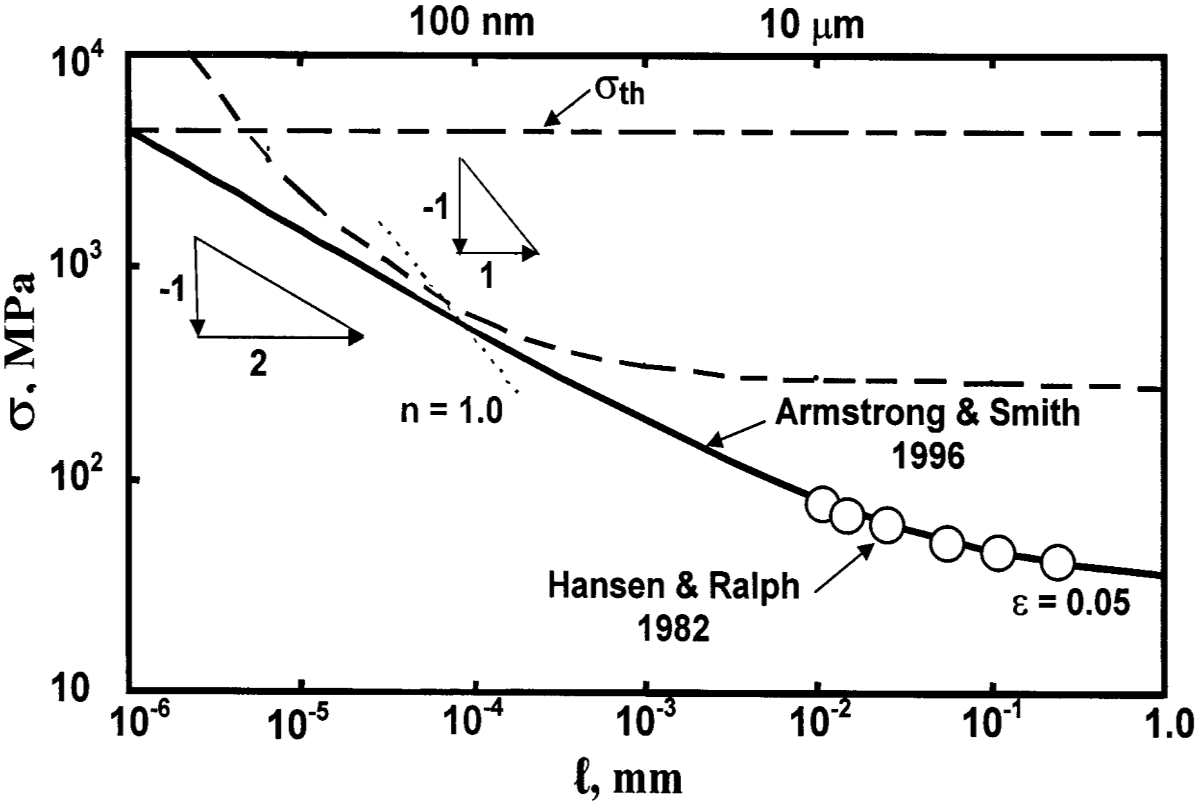
Log/log Hall-Petch Reference for Compiled Cu Strength vs. Grain Size Measurements

Reference: R.W. Armstrong, H. Conrad and F.R.N. Nabarro, in Mechanical Properties of Nanostructured Materials and Composites (eds. I. Ovid’ko et al.), Mater. Res. Soc. Symposium Proceedings, Vol. 791, pp. 69-77 (2004)



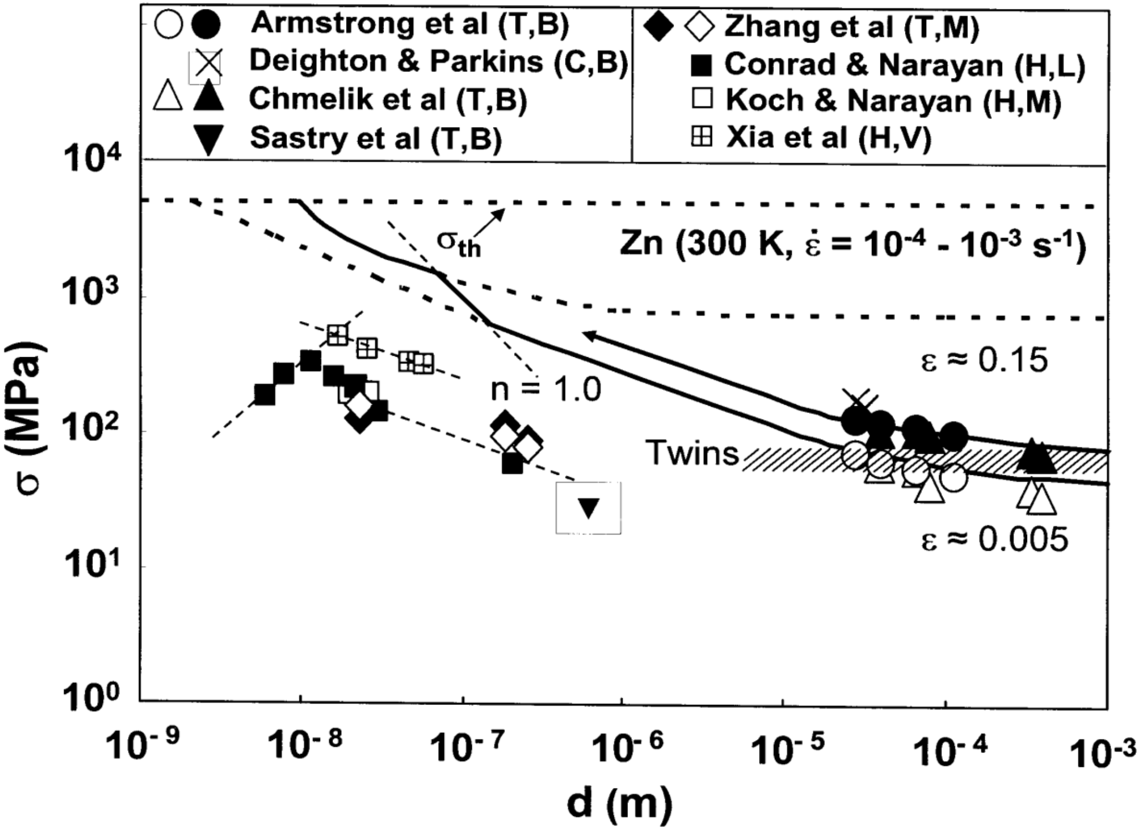
Hall-Petch Dislocation Pile-Up Transition to a Single Dislocation Loop Expanding Against the Grain Boundary Obstacle

Reference: R.W. Armstrong and P. Rodriguez, Philos. Mag. 86, 5787-5796 (2006); and, J.CM. Li and G.C.T. Liu, Philos. Mag, 15, 1059ff (1967)



Hall-Petch Application to Log/Log Compilation of Measurements on Zn

References: P. Rodriguez and R.W. Armstrong, (Indian) Bull. Mater. Sci., 29, 717-720 (2006); and, H. Conrad and J. Narayan, Acta Mater., 50, 5067-5078 (2002)

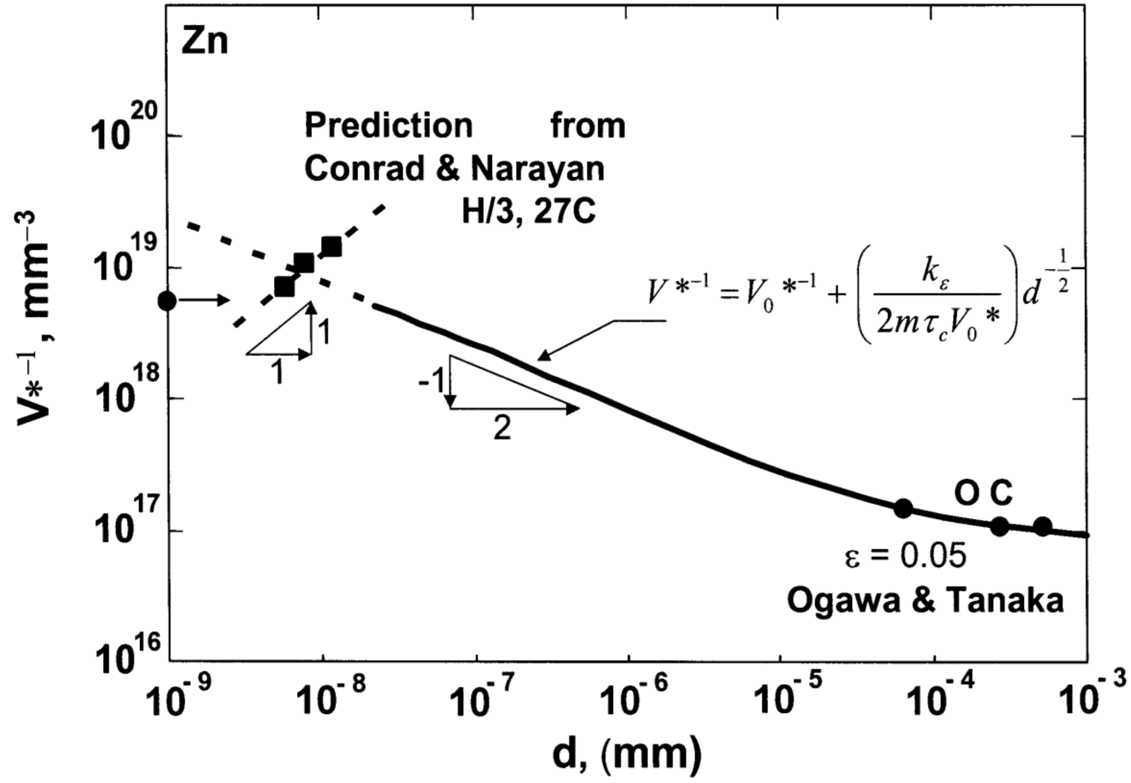


Comparison of Hall-Petch v^{*-1} and Creep-Based Grain Size Weakening Predictions

References: P. Rodriguez and R.W. Armstrong, (Indian) Bull. Mater. Sci., 29, 717-720 (2006); and, T.G. Langdon, J. Mater. Sci., 41, 597ff (2006)*

***$(d\varepsilon/dt) = (ADGb/k_BT)(b/d)^p(\sigma/G)^q$ for grain size weakening**

With **$p=q=1.0$, $v^{*-1} = \sigma/mk_BT$**



Computational equations for $\sigma = \sigma\{\varepsilon, T, (d\varepsilon/dt), \ell^{-1/2}\}$

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

$$v = v_0\mathbf{exp}[-(G_0 - \int A^* b d\tau_{Th})/kT] \quad \text{and} \quad v^* = A^* b = W_0/\tau_{Th}$$

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

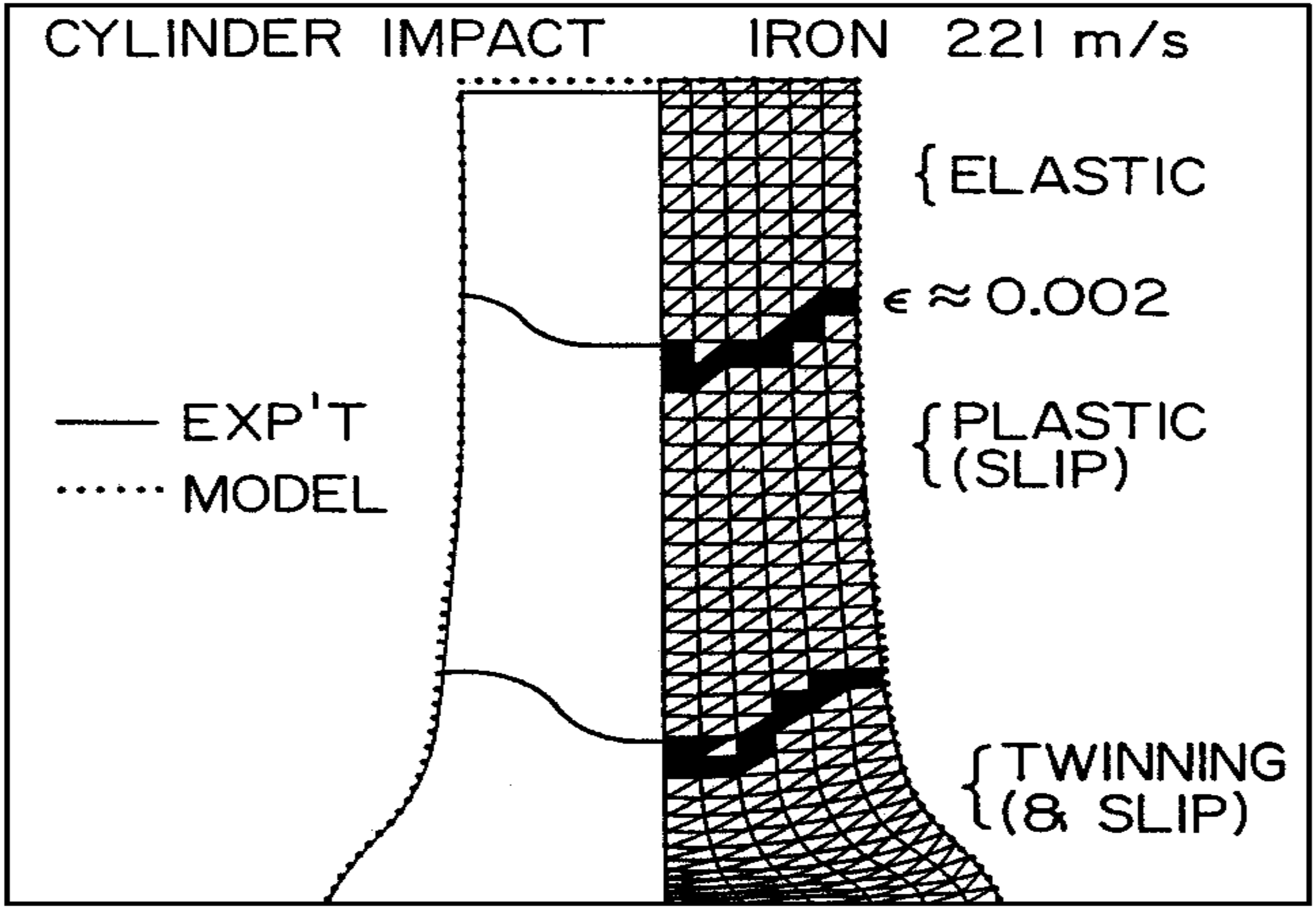
$$(\beta,\alpha) = (\beta_0,\alpha_0) - (\beta_1,\alpha_1)\mathbf{ln}(d\varepsilon/dt)$$

bcc case: $\alpha = \alpha_0 = \alpha_1 = 0$ fcc case: $B = 0;\ \beta = \beta_0 = \beta_1 = 0$

Thus on a TASRA basis, thermal activation is in the yield stress for bcc metals and alloys and is in the strain hardening for fcc metals and alloys.

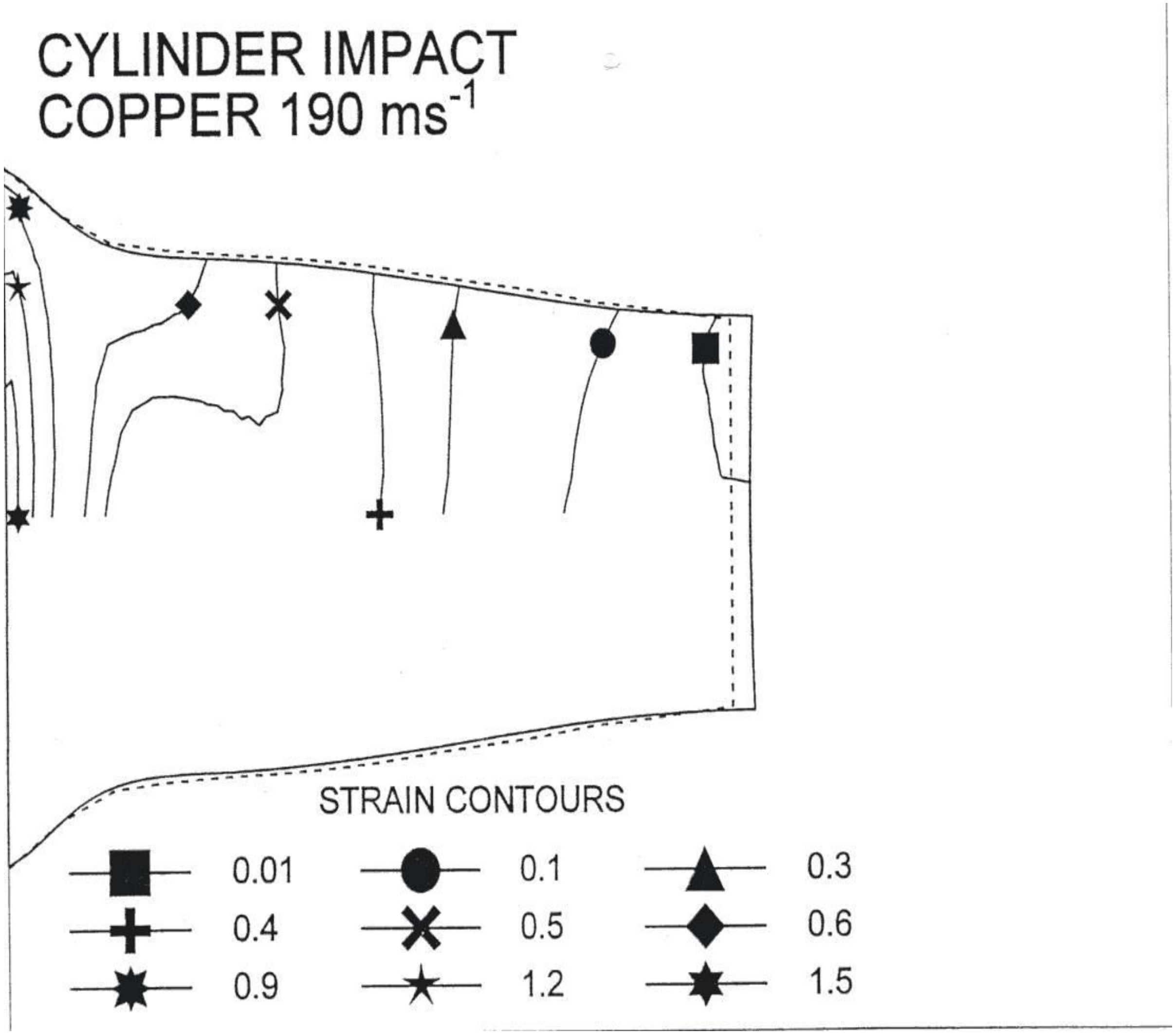
F.J. Zerilli and R.W. Armstrong, *J. Appl. Phys.* **61**, 1816-1825 (1987)
F.J. Zerilli and R.W. Armstrong, *J. Appl. Phys.* **68**, 1580-1591 (1990)
F.J. Zerilli, *Metall. Mater. Trans. A*, **35A**, 2547-2555 (2004)

Taylor-type impact result for Armco iron



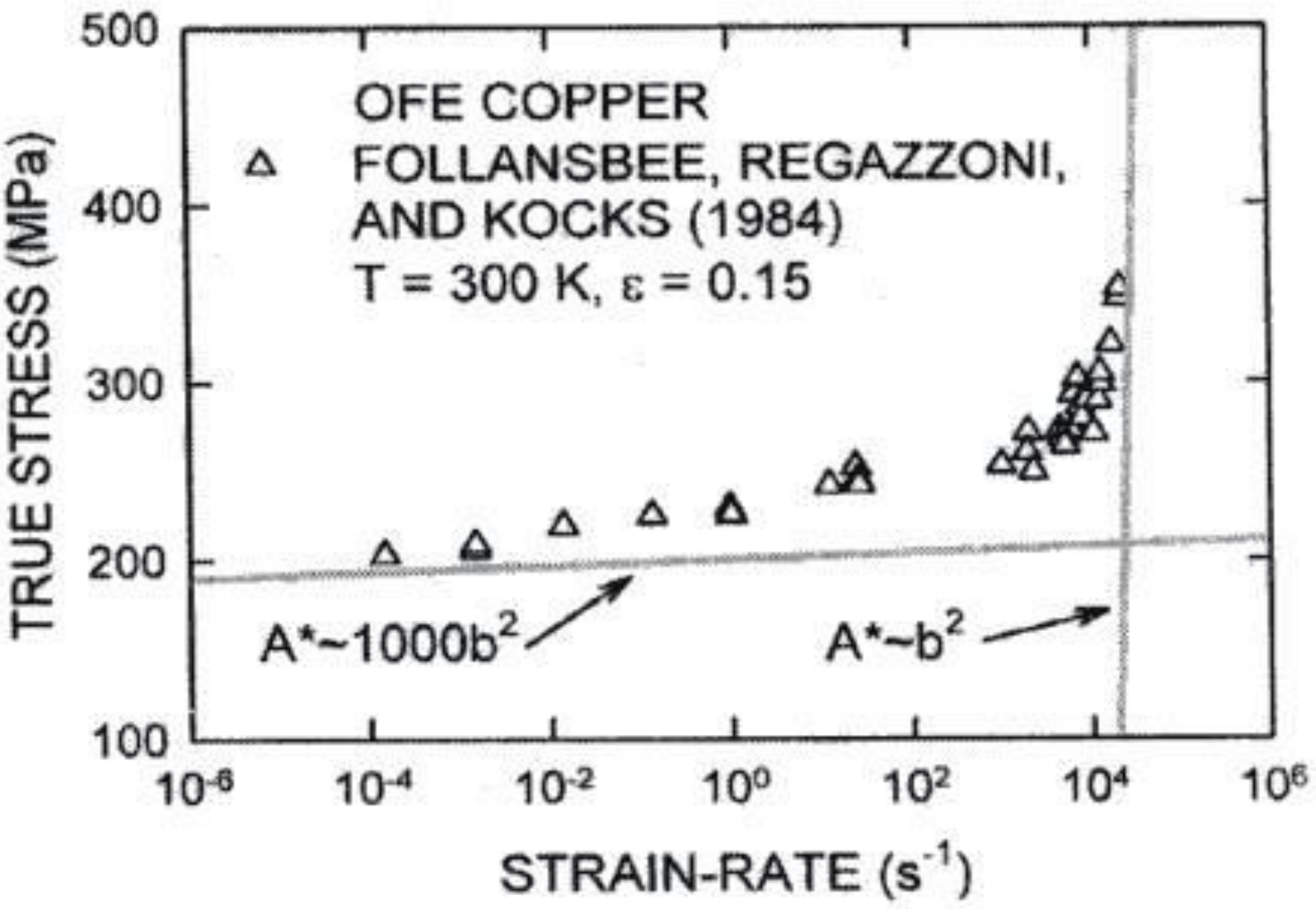
R.W. Armstrong and F.J. Zerilli, *J. de Phys.-Coll.,Fr,* **49**, C3-529 (1988), after measurements of G.R. Johnson and W.H. Cook, *Eng. Fract. Mech.,* **21**, 31 (1985)

Taylor-type impact result for copper



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

Activation volume asymptotes for copper



F.J. Zerilli and R.W. Armstrong, *Acta Mater.,* **40**, 1803 (1992) for drag; and, for generation, R.W. Armstrong, W. Arnold and F.J. Zerilli, *Metall. Mater. Trans. A*, **38A**, 2605-2610 (2007)

Transition from dislocation velocity control to dislocation generation control

For dislocation velocity control:

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

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

in which

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

For dislocation generation control:

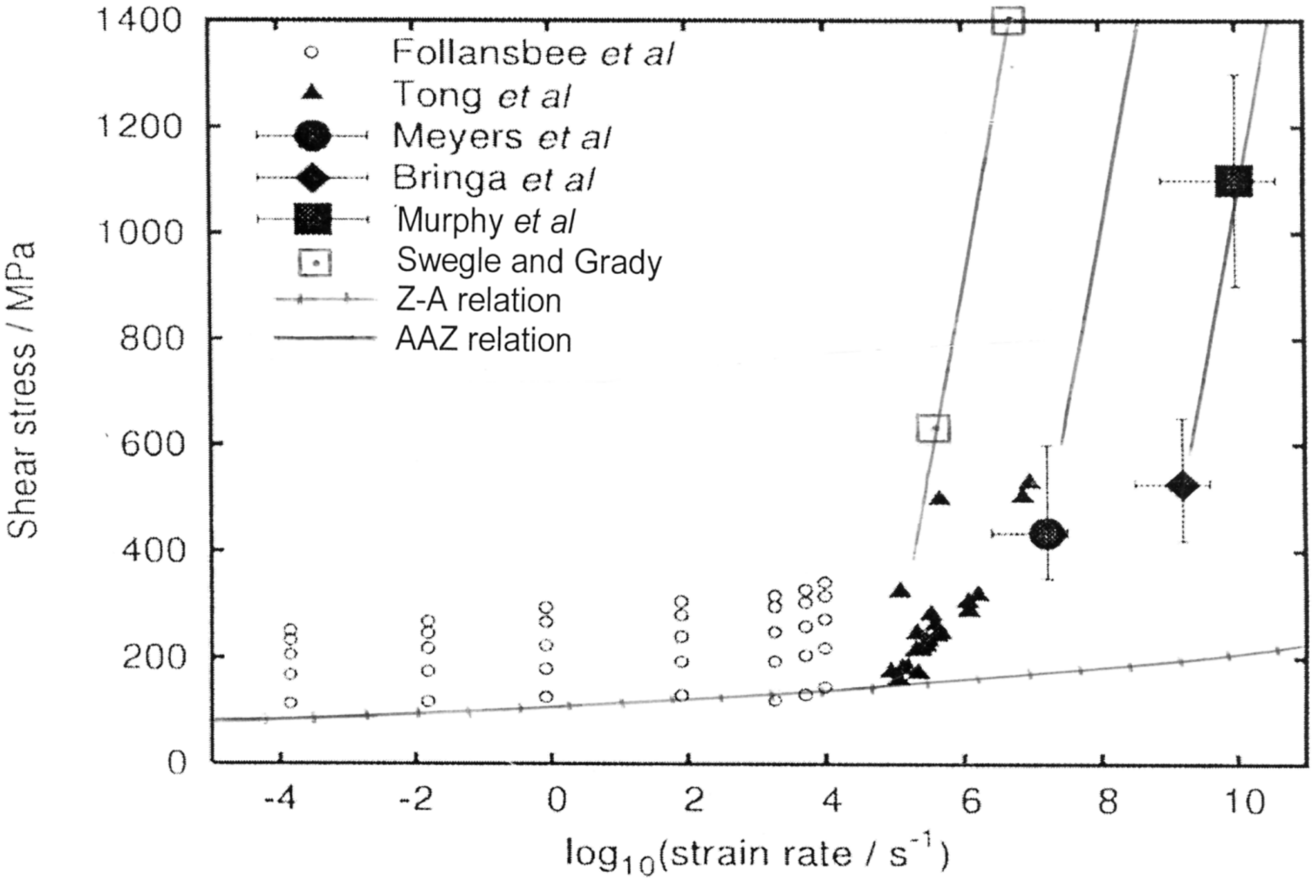
$$(d\varepsilon/dt) = (1/m)b(d\rho/dt)\Delta x_d$$

in which, at limiting small value of $v^* \sim b^3$, and $m = 2$

$$\sigma_{Th} = (2G_{0G}/v^*) - (2kT/v^*)\,[\mathbf{ln}\{(d\varepsilon/dt)_0/(d\varepsilon/dt)\}]$$

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

Copper deformations extending to shocking rates



W.J. Murphy *et al., J. Phys.: Condens. Matter*, **22**, 065404 (2010); R.W. Armstrong and F.J. Zerilli. *J. Phys. D: Appl. Phys.,* **43**, 492002 (2010)

TASRA with dislocation drag:

$$v = d/(t + t_d); \ (d/t_d) = b\tau/c_0; \ (d/t) = v_0 \mathbf{exp}(-G/kT)$$

The resident dislocation density is required to “carry the load”, and because ρ_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

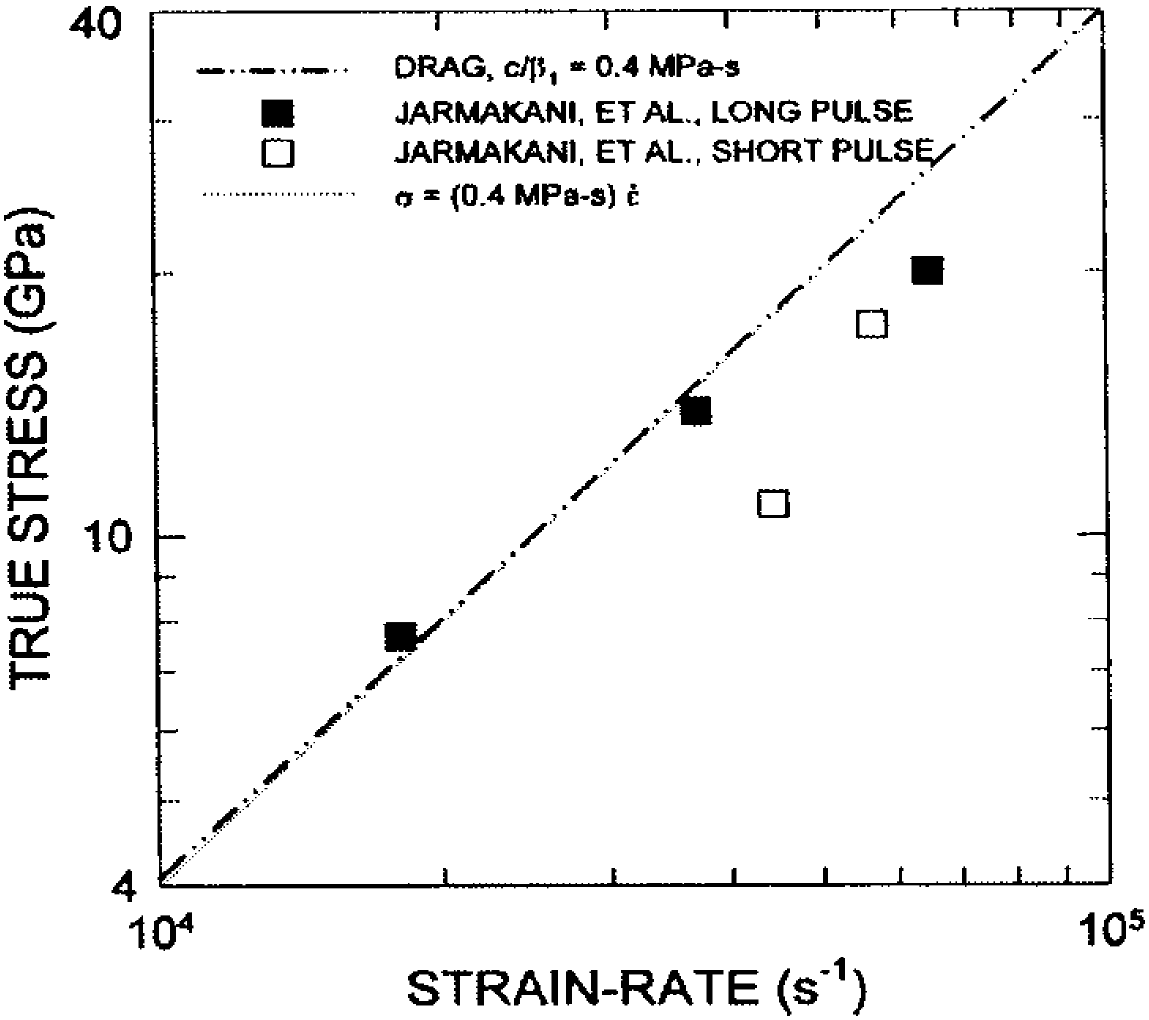
$$c = c_0 m^2 \beta_1/\rho b^2 \quad \text{and} \quad b\tau_{Th} = c_0 v.$$

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. Hall-Petch, dislocation pile-up interpreted, grain size results have been evaluated for various metals over a large range in grain diameters, temperatures, and strain rates; for example, for copper over 4.0 nm $\leq \ell \leq$ 0.25 mm, a factor of ~60,000X.

1.1. H-P k_{ε} values for copper are reported over a range of temperatures from 4.2 to 673 K.

1.2. H-P k_{ε} values for copper are reported for $10^{-4} \leq (d\varepsilon/dt) \leq 10^{3}$ s^{-1}.

2. Thermally-activated (viscoplastic) strength levels have been evaluated at conventional stress-strain, split Hopkinson pressure bar, Taylor type cylinder impact test, shock, and shockless isentropic compression tests that provide for discrimination between control by dislocation velocity, with and without drag influence, and dislocation generation; for copper, 40 MPa $\leq \sigma_{\varepsilon} \leq$ 20 GPa, a factor of 500X, corresponding to reported strain rates of $10^{-4} \leq (d\varepsilon/dt) \leq \sim 10^{10}$ s^{-1}.