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MICROSTRUCTURAL/DISLOCATION MECHANICS ASPECTS OF SHEAR BANDING IN POLYCRYSTALS

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ABSTRACT

At increased tensile strain rates or decreased test temperatures, face-centered-cubic (fcc) metals show an increased uniform strain to the maximum load point, in contrast to the decreased uniform strain behavior exhibited by body-centered-cubic (bcc) metals under the same conditions. The opposite tensile plastic instability behaviors of the two structure-types are explained on a thermal activation/strain rate analysis (TASRA) basis in terms of strain-dependent dislocation "forest" intersections controlling the fcc thermal component of stress as compared with a strain-independent intrinsic Peierls stress for individual dislocations being responsible for the relatively larger bcc thermal component of stress. Bcc metals are differentiated from fcc metals, also, by showing an initial discontinuous yield point behavior that is increasingly pronounced as the polycrystal grain size is smaller. The yield point behavior is explained by the breakthroughs at grain boundaries of blocked dislocation pile-ups in slip bands. The behavior is gauged by the microstructural stress intensity value determined from the dependence of yield stress on the reciprocal square root of the average polycrystal grain diameter. Substantial temperature rises are calculated on a dislocation pile-up avalanche basis for this instability behavior in metallic, ionic, and energetic (explosive) materials.

Microstructures and Dislocation Pile-Ups

Figure 1 relates to a number of grain morphology and dislocation modeling considerations (1-4). Réaumur, in 1722, and Grignon, fifty-three years later in 1775, reported from observing iron cleavage facet reflections on fractured steel specimens that improved mechanical properties were obtained with finer grained microstructures (1). The topology of grain structures composing a polycrystalline aggregate remains a subject of interest to researchers today, for one reason because the dislocation slip and deformation twinning mechanisms responsible for permanent deformation and fracturing are tied to the crystal axes within an individual grain (2) and are limited in movement to the areal extent of planes confined within the grain perimeter (3). A recent consideration has involved the role of dislocation pile-ups in effecting a transition from ductile fracturing to cleavage initiation at particle clumps in structural steel materials (4).

Discontinuous load drops obtained in titanium (5) and steel (6) materials tested at liquid helium temperature are shown in Figure 2. The load drops are attributed to deformation twinning "bursts" that were initiated at micro-slip dislocation pile-ups. Figure 3 gives a sampling of mathematical descriptions of dislocation pile-up behavior, including static and dynamic considerations. The yield and flow strength/microstructural consequences of the pile-up description of slip band behavior have been reviewed (7). Figure 4 relates to the predicted dependence of yield and fracture strength on reciprocal square root of interlamellar spacing for unidirectionally-solidified intermetallic compound materials designed for use in gas turbine engines. The low values of fracture strain preceding fracture at ambient temperature are attributed to the relatively large value of the microstructural stress intensity determined from the slope dependence that is shown. The experimental slope value is near to the computed theoretical limit for brittle fracturing.

The Thermal Activation/Strain Rate Analysis (TASRA)

Zener and Hollomon (8) described the coupled temperature and strain rate dependence of the flow stresses of various steel materials in their pioneering investigation of shear banding produced by a blunt-edged punch. Zerilli and Armstrong (9) have given a dislocation mechanics description of the thermally-activated flow stress behavior for steel and related body-centered-cubic (bcc) metals as compared with the quite different behavior exhibited by face-centered-cubic (fcc) metals such as copper. The TASRA equations, including the strain rate dependent activation area expression, are combined with the Hall-Petch stress/grain size equation in Figure 5 as applicable to the bcc and fcc cases. The bcc case involves a strain-independent TASRA description of the Peierls friction stress for individual dislocation motion as compared with strain-dependent dislocation "forest" intersections controlling the thermal friction stress in the fcc case.

The fcc flow stress equation is shown again in Figure 6 that also includes experimental results obtained on copper over a range of temperatures, strain rate and grain size by Carreker and Hibbard (10). The increased temperature dependence of the tensile strength over that of the yield stress, at all grain sizes, and the strain rate dependence of the flow stress at two grain sizes is in agreement with the combined TASRA and grain size prediction, in this case including a TASRA contribution to the microstructural stress intensity. Figure 7 shows counterpart temperature and strain rate measurements reported by Marchand and Duffy (11) for a structural steel. The roughly parallel shift of the flow stress curves at different temperatures, for a strain rate of 1000 per second, and at different strains are in agreement with the bcc constitutive equation. Both equations have been usefully applied to predicting independent measurements of the full deformation shapes of solid cylinders impacted onto essentially rigid targets.

Plastic Instability for BCC and FCC Metals

The plastic instability property of the bcc and fcc equations has been analyzed from the viewpoint of obtaining material constants for the strain hardening behavior from reference tests and comparing the maximum load point strain conditions for the two structure types. Figure 8 shows the form of the equations from which the effects of temperature and, implicitly, of strain rate produce opposite influences on the uniform strain to the maximum load point for bcc and fcc structures (12).

Figures 9 and 10 show an example of reference experimental and fitted stress/strain curves for tantalum material, including the maximum load point strain dependence that has been described (13). The constitutive equation constants were employed then to compute the solid cylinder impact results that are shown to be in agreement with experiment in Figure 11. The opposite dependencies predicted for bcc tantalum and Armco iron as compared with fcc copper are shown in Figure 12. Petch and Armstrong (14) have given a tabulation of measurements for various metals and alloys showing agreement with these results. Thus, this average constitutive equation description of strain rate and temperature influences on the deformation behavior of bcc and fcc metals indicates on a uniform strain to the maximum load point basis that the former structure type should be relatively shear band prone.

Dislocation Pile-Up Initiation of Shear Banding?

The discontinuous yield point behavior of steel that is associated with the propagation of Luders' bands was noted in the pioneering work of Zener and Hollomon (8). Petch (15) has given a recent review of the behavior that is increasingly pronounced as the polycrystal grain size is smaller, reflecting the increasing importance of dislocation pile-ups and the microstructural stress intensity term in the Hall-Petch polycrystal flow stress equation. Armstrong, Coffey and Elban (16) have proposed that very appreciable heating can occur locally when individual dislocation pile-ups are released from their blocking obstacles, particularly at stress intensity values near to the theoretical limit for cracking.

The model for this behavior is indicated in Figure 13 along with an equation for the limiting temperature rise that could be expected. In this case, the ratio of the microstructural stress intensity and the thermal conductivity provides an index of a material susceptibility to such heating (17). The results on discontinuous load drops shown in Figure 2 seem in line with the proposed behavior. New results obtained on shear banding in Ti6Al4V alloy, as indicated in Figure 14, show it to be even more sensitive to shear banding than titanium (18). Current research involves the application of this proposal to understanding the drop-weight impact sensitivity of energetic (explosive) crystals where an effect of crystal size as shown in Figure 15 has been accounted for on a dislocation pile-up avalanche basis (19,20).

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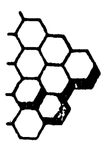
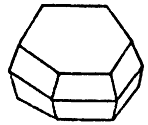
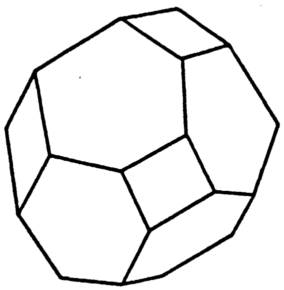


hexahedral Fe crystals

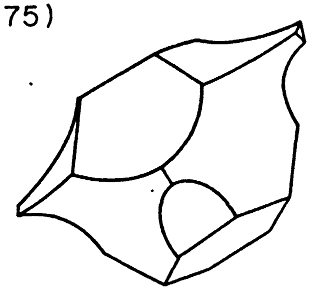


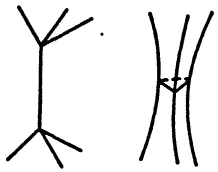
decatetrahedral-hexagon

Grignon (1775)

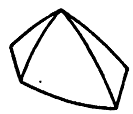


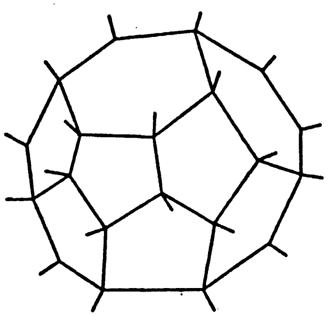
tetrakaidecahedron



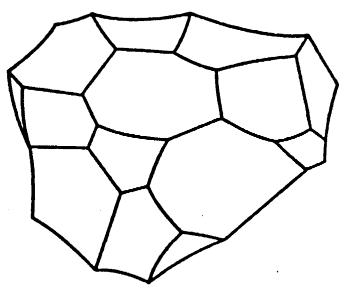


Smith (1953)



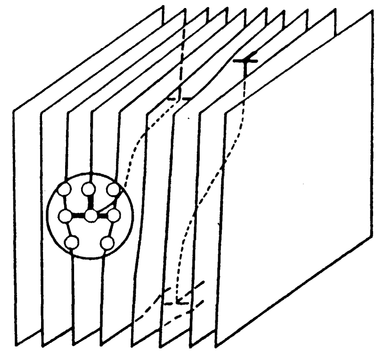


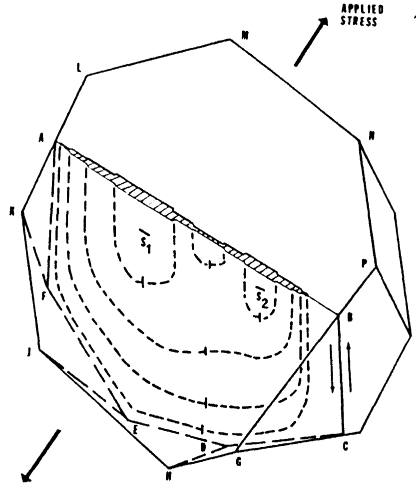
average grain

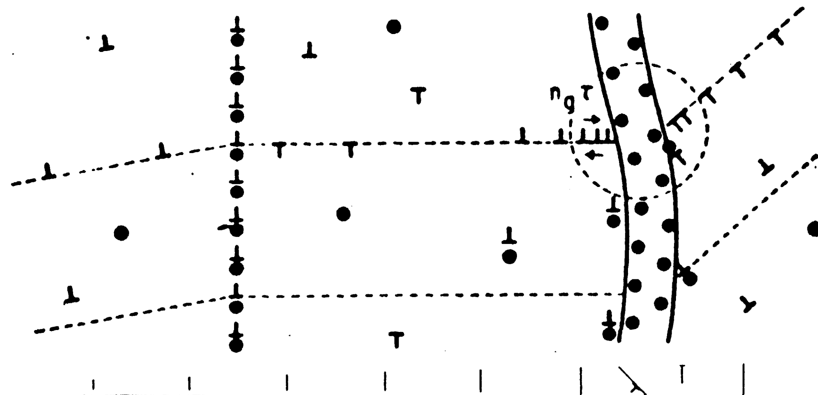


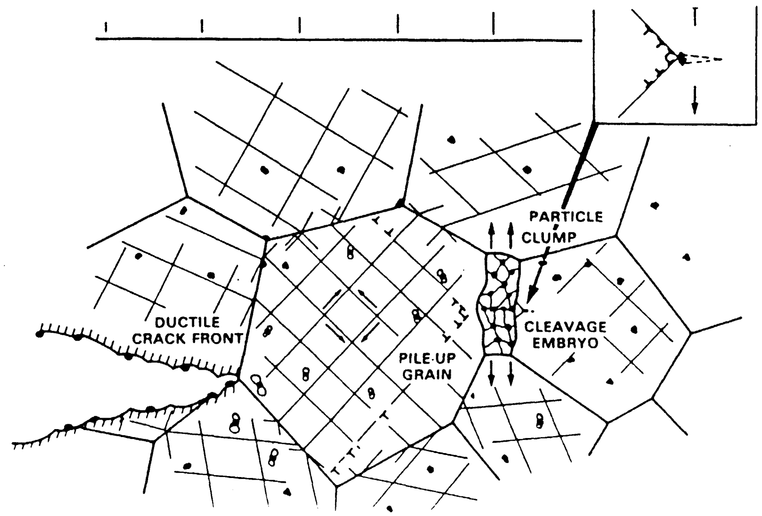
simple and complex grains

Rhines, Craig and DeHoff (1974)









Discontinuous Twinning of Titanium at 4.2 K

N. M. MADHAVA AND R. W. ARMSTRONG

METALLURGICAL TRANSACTIONS VOLUME 5, JUNE 1974–1517

Discontinuous Twinning during Essentially Elastic Compression of Steel at 4·2°K †

N. M. MADHAVA, P. J. WORTHINGTON‡ and R. W. ARMSTRONG

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PHILOSOPHICAL MAGAZINE, Vol. 25, No. 2, p. 519, February 1972

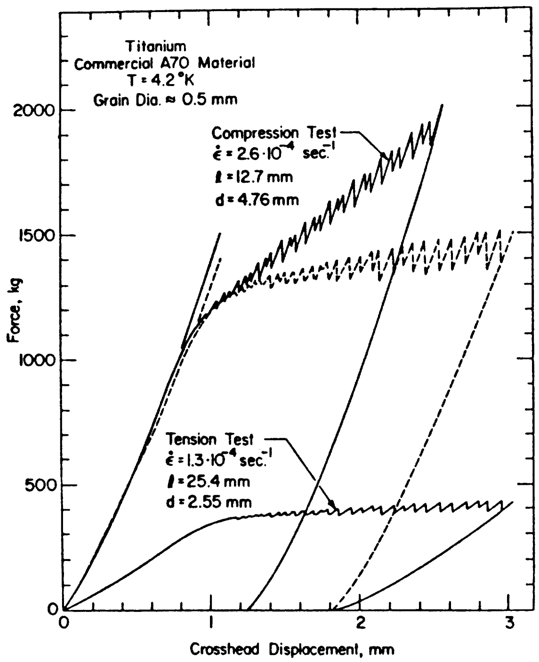
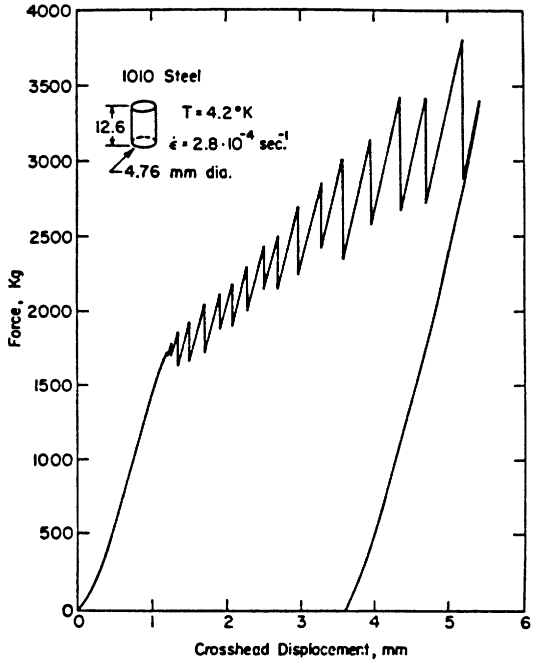
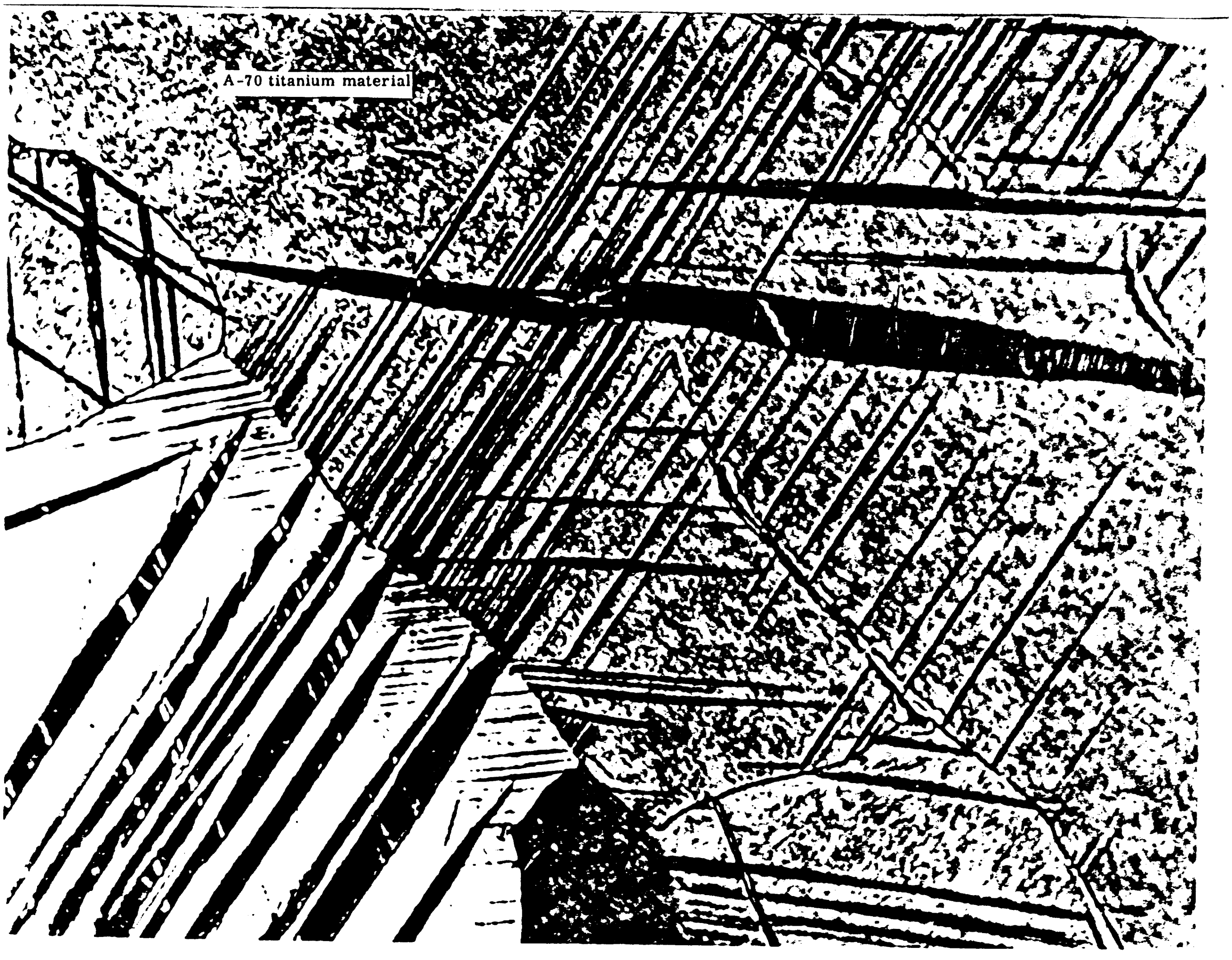


Fig. 1—Tension and compression force-displacement curves for large grain A-70 titanium material.



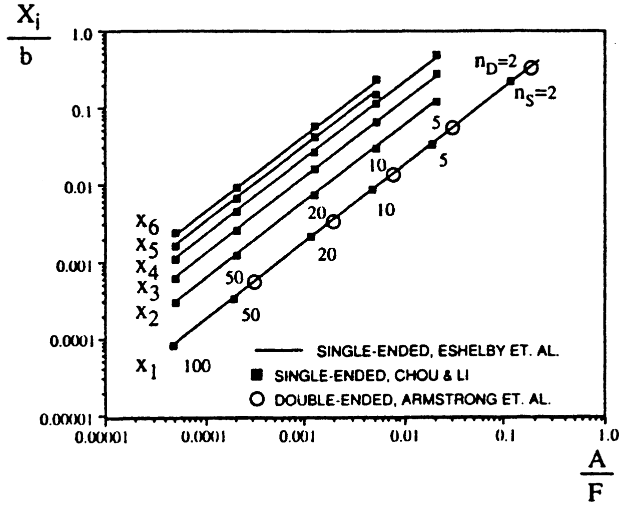
A typical force/crosshead displacement curve.



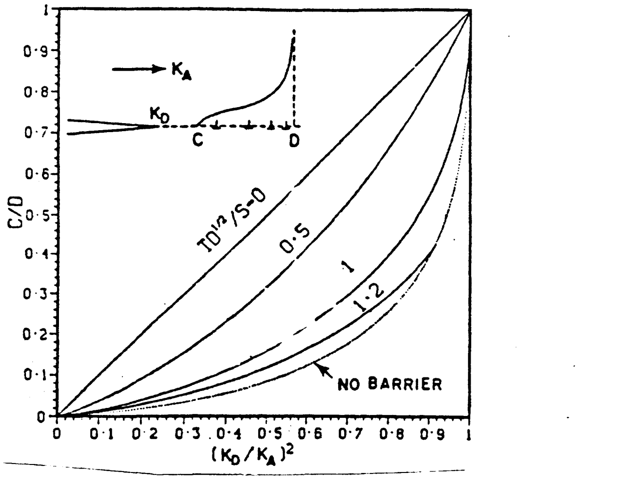
DISLOCATION PILE-UP DESCRIPTIONS OF SHEAR BANDING

I. Static pile-up results

J.C.M. Li and Y.T. Chou, "The Role of Dislocations in the Flow Stress/Grain Size Relationships", Metallurgical Transactions, 1, 1145 (1970); Wen-Lan Li and J.C.M. Li, "The Effect of Grain Size on Fracture Toughness", Philosophical Magazine, A59, 1245 (1989); Q. Gao and H.W. Liu, "Characterization of the Tip Field of a Discrete Dislocation Pile-up for the Development of Physically Based Micromechanics", Metallurgical Transactions, 21A, 2087 (1990).



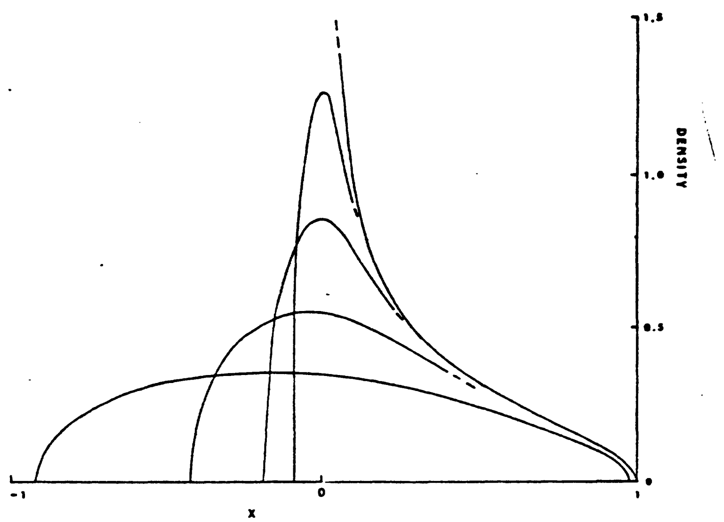
The position, X_i, of the i-th dislocation in a pileup.



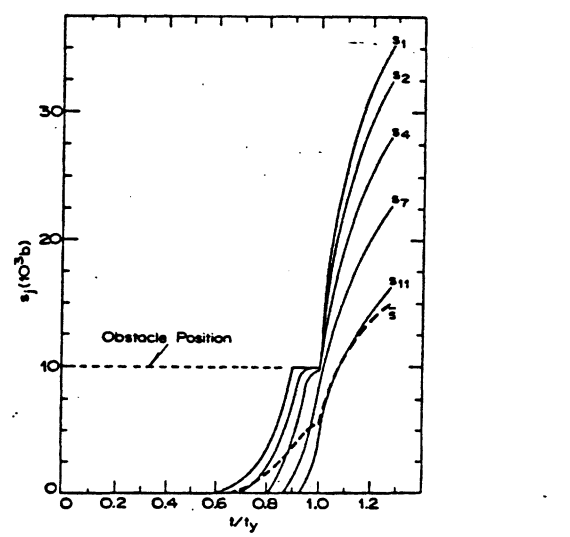
Dislocation-free zone at the crack tip; the effect of lattice friction and barrier distance.

II. Dynamic pile-up results

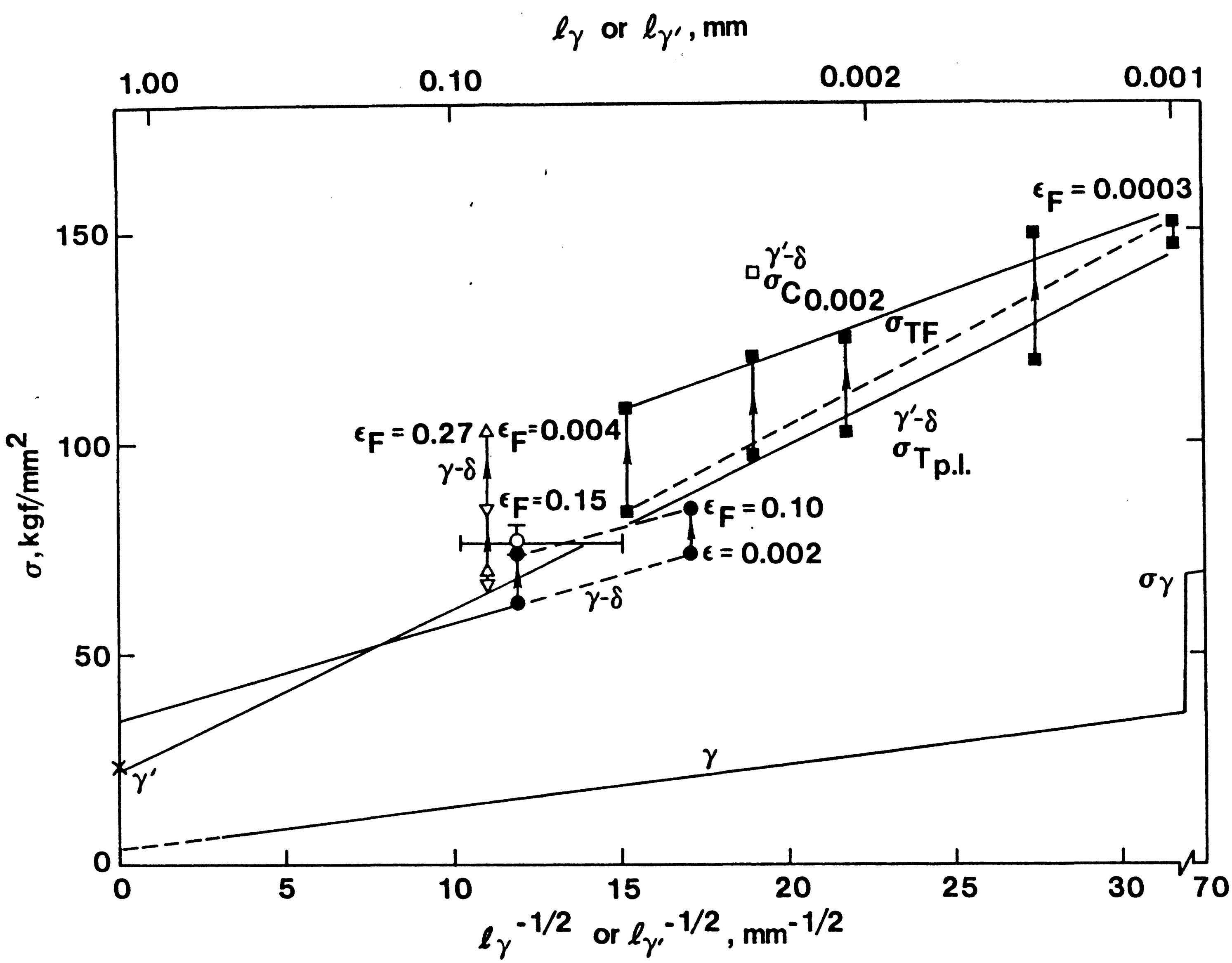
A.K. Head, "Dislocation Group Dynamics VI. The Release of a Pile-up", Philosophical Magazine , 27, 531 (1973); F.P. Gerstle and G.J. Dvorak, "Dynamic Formation and Release of a Dislocation Pile-up Against a Viscous Obstacle", Philosophical Magazine, 29, 1337 (1974); Hilary Ockendon and J.R. Ockendon, "Dynamic Dislocation Pile-ups", Philosophical Magazine, 47A, 707 (1983).



The shape of the dislocation distribution as it moves from right to left, at times $T=0$, 0·01, 0·03, 0·1 and 0·3.



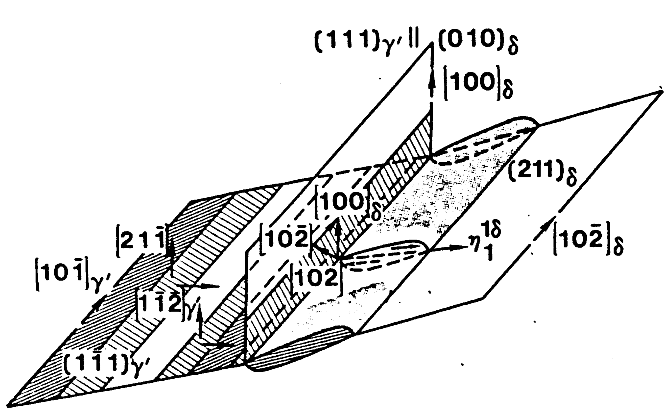
Positions s_i of individual dislocations during a constant strain-rate test ($\dot{\epsilon} = 100$ sec
$t_y = 42{\cdot}6\ \mu$sec).



$(211)_\delta, \eta_1^{1\delta}$ twin nucleated by $(1\bar{1}1)_{\gamma'}\,[10\bar{1}]_{\gamma'}$ slip

Dislocation reaction:

$1/2\,[10\bar{1}]_{\gamma'} - 1/6\,[21\bar{1}]_{\gamma'} \approx \eta_1^{1\delta} - 1/7\ \ (1/2\ [100]_\delta)$



Hall-Petch k_ϵ values for γ or γ'-δ eutectics versus single phase ordered or disordered $L1_2$ structures

Reference	Material	k_ϵ, kgf/mm$^{3/2}$	
		Ordered	Disordered
1	Ni_3Al-Ni_3Nb (γ'- δ) eutectic	3.9	–
2	Ni{Al}- Ni_3Nb (γ - δ) eutectic	–	~2.0
3	Ni_3Mn	4.7	2.8
4	Ni_3Fe	4.0	3.0

References: 1) Thompson, George & Breinan (1973);
2) Thompson & Lemkey (1974);
3) Johnston, Davies & Stoloff (1965);
4) Arko & Liu (1971)

$$\dot{\gamma} = Nbv_o e^{-\frac{G_o}{kT} + \frac{1}{kT}\int_{\tau_{Th}^o}^{\tau_{Th}} A^* b \, d\tau'_{Th}}$$

$$\sigma_y = m[\tau_G + \tau_{Th}] + k\ell^{-1/2}$$

$$\varepsilon = \gamma/m \quad , \sigma_o = m[\tau_G + \tau_{Th}]$$

$$\left(\frac{\partial \ln \dot{\gamma}}{\partial \tau_{Th}}\right)_T = \frac{A^* b}{kT}$$

Experiment:

$$A^* b = mkT\left(\frac{\Delta \ln \dot{\varepsilon}}{\Delta \sigma}\right)_T = \frac{W_o}{\tau_{Th}}$$

$$\tau_{Th} = (\tau_{Th}^o e^{G_o/W_o}) e^{(kT/W_o)\ln(\dot{\gamma}/\dot{\gamma}_o)}$$

$$\sigma = B_o e^{-\beta T} \quad , \beta = \beta_o - \beta_1 \ln \dot{\varepsilon}$$

bcc case:

$$A^* \neq A^*\{\varepsilon\} \quad , 10b^2 \leq A^* \leq 1000b^2$$

$$\sigma = \sigma_G + B_o e^{-\beta_o T + \beta_1 T \ln \dot{\varepsilon}} + K\varepsilon^n + k\ell^{-1/2}$$

$$T = 0 \, , \; B_o = mG_o/\langle A \rangle_o b$$

fcc case:

$$A^* = A^*\{\varepsilon\} = db/2$$

$$\sigma_o \simeq \sigma_o'(b/d) \simeq \sigma_o'' \varepsilon^{1/2}$$

$$\langle A \rangle_o \approx A_o \varepsilon^{-1/2}$$

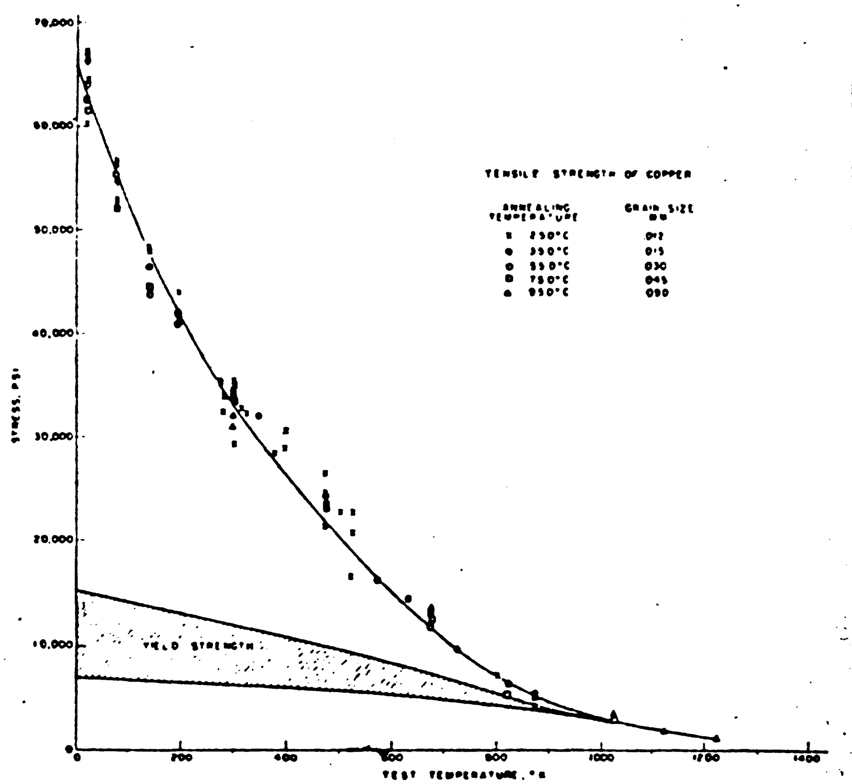
$$B_o = B_1 \varepsilon^{1/2}$$

$$\sigma = \sigma_G + B_1 \varepsilon^{1/2} e^{-\beta_o T + \beta_1 T \ln \dot{\varepsilon}} + k\ell^{-1/2}$$

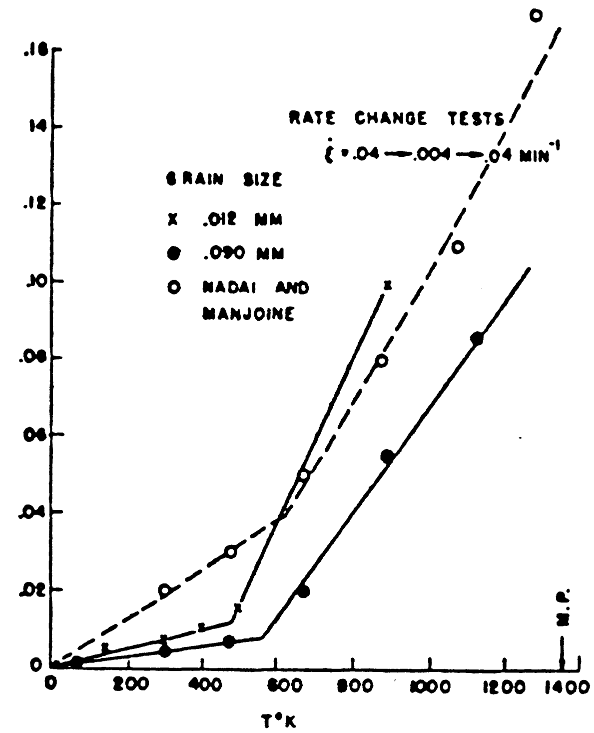
TENSILE DEFORMATION OF HIGH-PURITY COPPER AS A FUNCTION OF TEMPERATURE, STRAIN RATE, AND GRAIN SIZE

R. P. CARREKER, Jr. and W. R. HIBBARD, Jr.

ACTA METALLURGICA, VOL. 1, NOV. 1953



Tensile strength of copper as a function of temperature for each of several grain sizes.



$$\sigma = \sigma_{0_G} + C_2\epsilon^{1/2}\exp\left(-C_3T + C_4T\ln\dot{\epsilon}\right) + k\ell^{-1/2}$$

$$n \equiv \frac{1}{\sigma}\left(\frac{\partial\sigma}{\partial\ln\dot{\epsilon}}\right)_T .$$

For $\left(k\ell^{-1/2}/\sigma_0\right) < 1.0$,

$$n = \frac{RT}{\sigma_0 v_0^*}\left[1 + \left\{\left(\frac{1}{2m_T\tau_c}\right)\left(\frac{v_0^*}{v_c^*}\right) - \frac{1}{\sigma_0}\right\}k\ell^{-1/2}\right]$$

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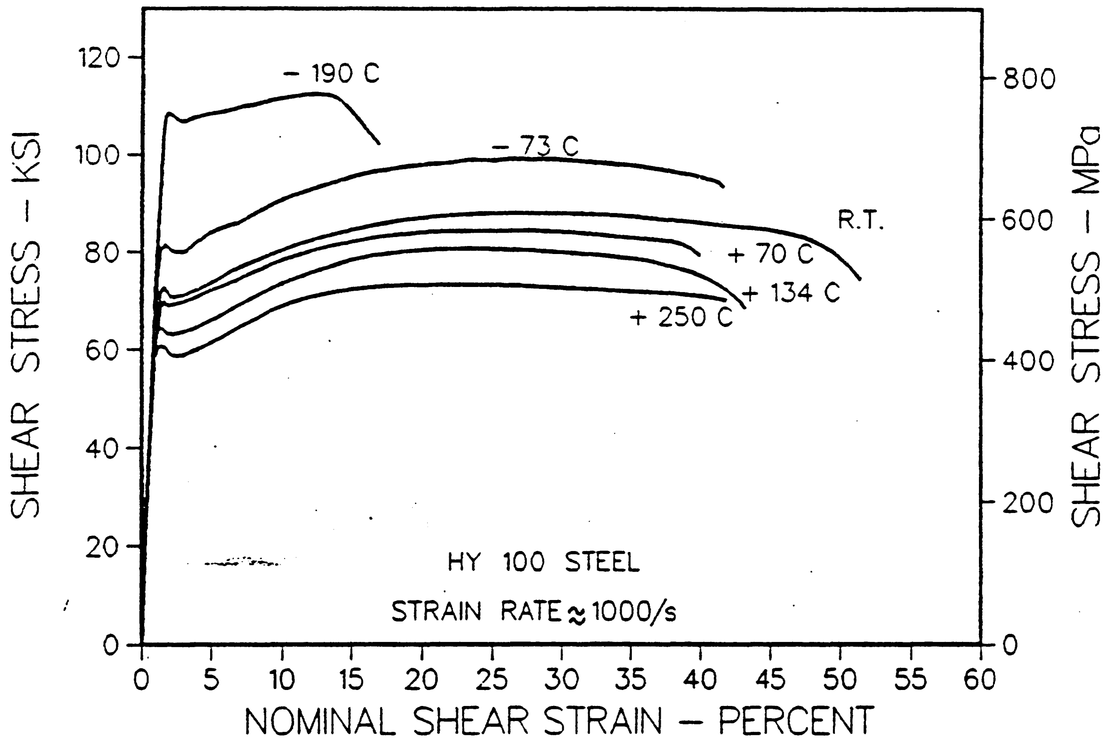
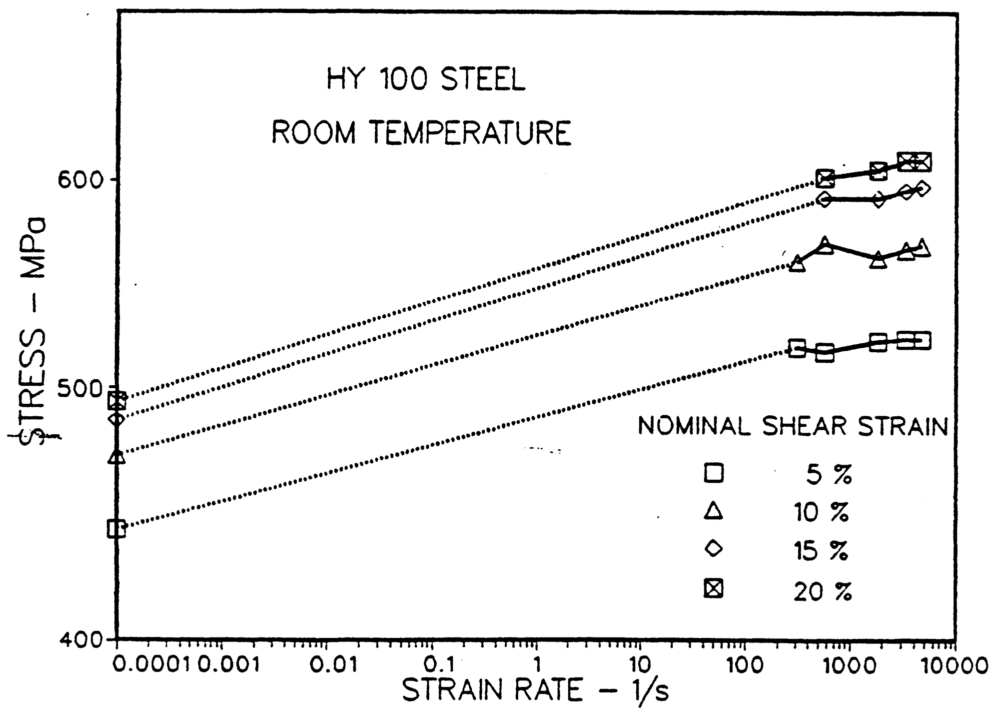
AN EXPERIMENTAL STUDY OF THE FORMATION PROCESS OF ADIABATIC SHEAR BANDS IN A STRUCTURAL STEEL

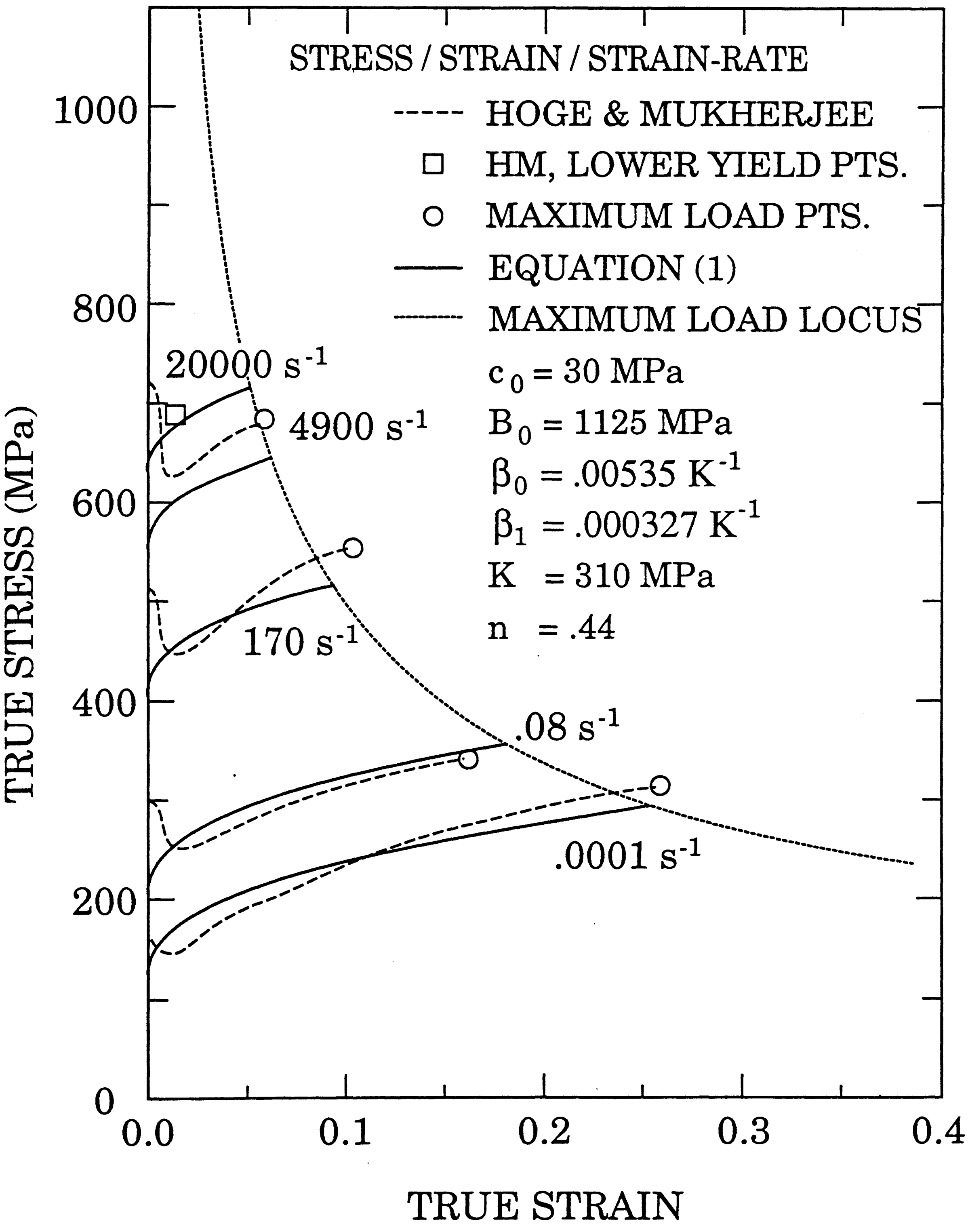
Office of Naval Research
Contract No. N00014-85-K-0597

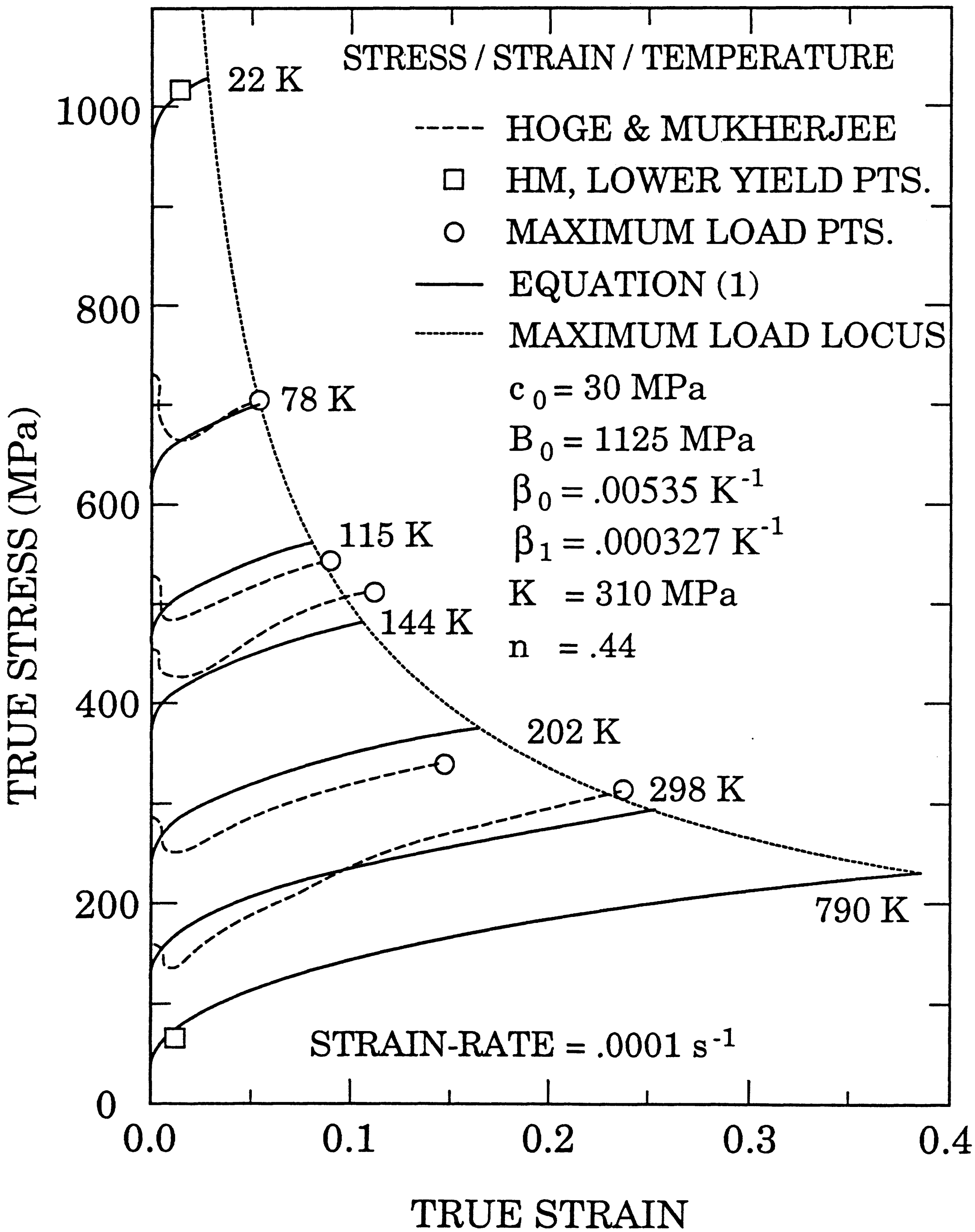
Materials Research Laboratory
Grant DMR-8316893

April, 1987

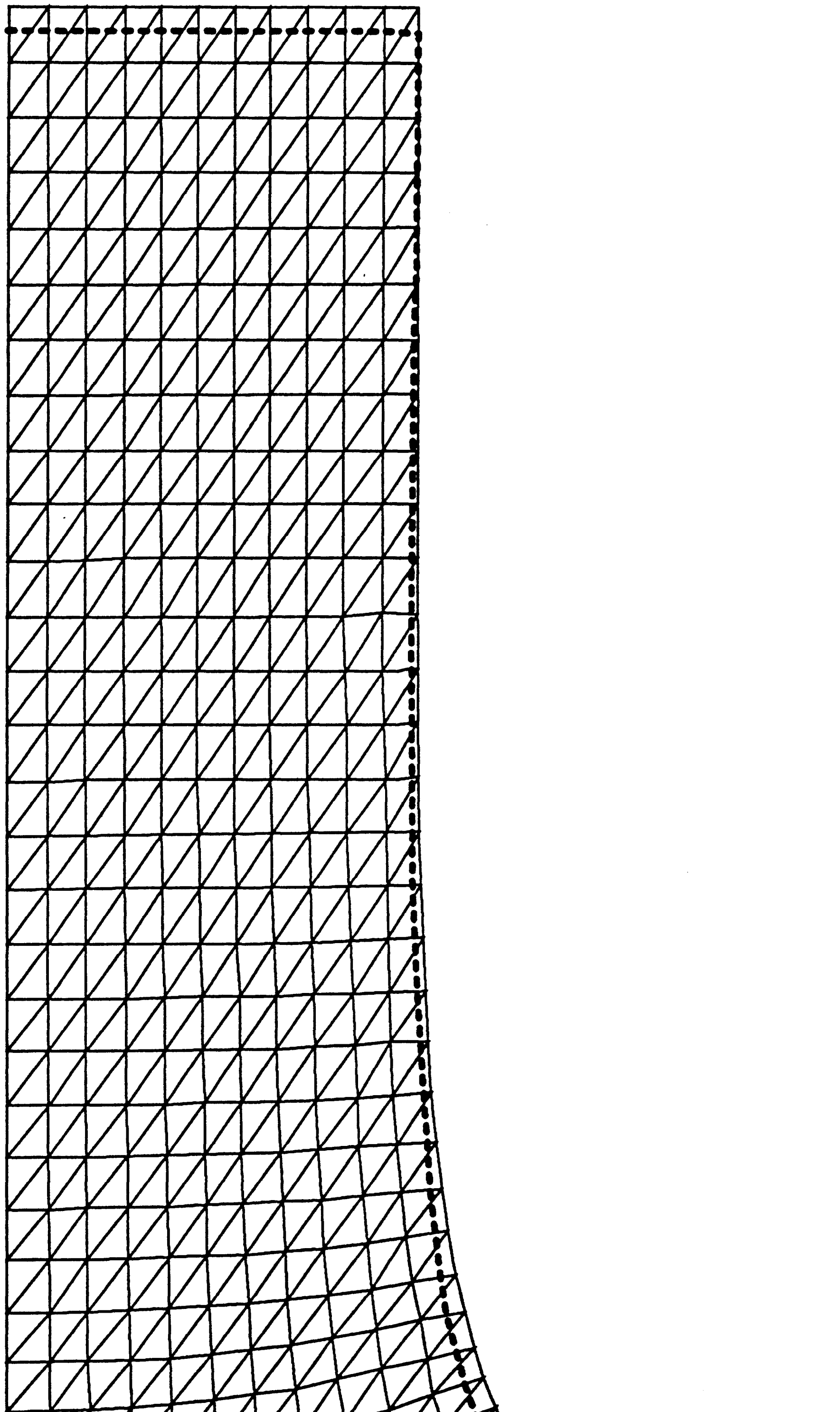


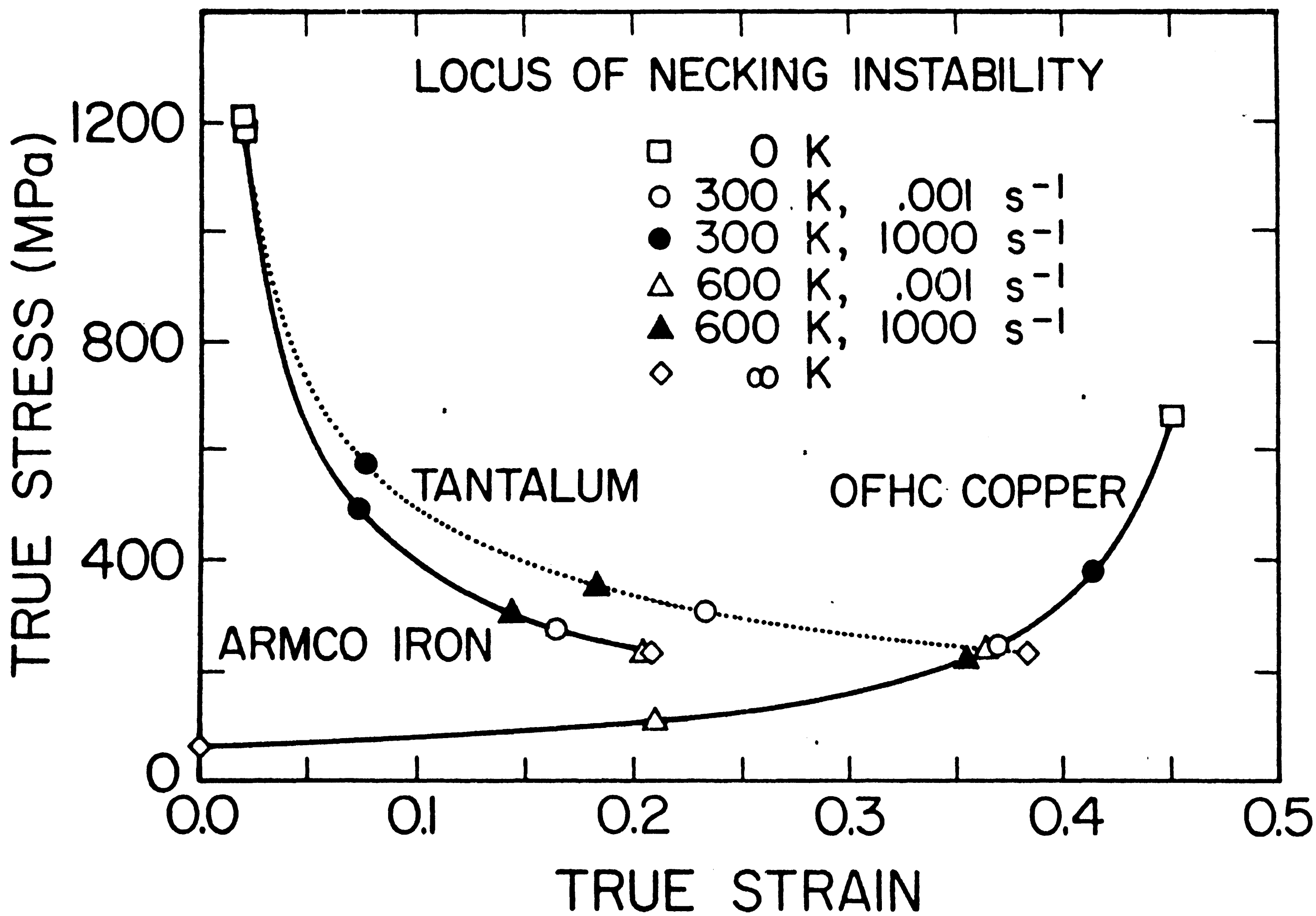



STRESS / STRAIN / STRAIN-RATE
HOGE & MUKHERJEE
HM, LOWER YIELD PTS.
MAXIMUM LOAD PTS.
EQUATION (1)
MAXIMUM LOAD LOCUS
c_0 = 30 MPa
B_0 = 1125 MPa
β_0 = .00535 K^{-1}
β_1 = .000327 K^{-1}
K = 310 MPa
n = .44
20000 s^{-1}
4900 s^{-1}
170 s^{-1}
.08 s^{-1}
.0001 s^{-1}
TRUE STRESS (MPa)
TRUE STRAIN
0
200
400
600
800
1000
0.0
0.1
0.2
0.3
0.4



STRESS / STRAIN / TEMPERATURE
HOGE & MUKHERJEE
HM, LOWER YIELD PTS.
MAXIMUM LOAD PTS.
EQUATION (1)
MAXIMUM LOAD LOCUS
$c_0 = 30$ MPa
$B_0 = 1125$ MPa
$\beta_0 = .00535\ K^{-1}$
$\beta_1 = .000327\ K^{-1}$
K = 310 MPa
n = .44
22 K
78 K
115 K
144 K
202 K
298 K
790 K
STRAIN-RATE = $.0001\ s^{-1}$
TRUE STRESS (MPa)
TRUE STRAIN
0
200
400
600
800
1000
0.0
0.1
0.2
0.3
0.4





LOCUS OF NECKING INSTABILITY
0 K
300 K, .001 s⁻¹
300 K, 1000 s⁻¹
600 K, .001 s⁻¹
600 K, 1000 s⁻¹
∞ K
TANTALUM
OFHC COPPER
ARMCO IRON
TRUE STRESS (MPa)
0
400
800
1200
0.0
0.1
0.2
0.3
0.4
0.5
TRUE STRAIN

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ADIABATIC HEATING AT A DISLOCATION PILE-UP AVALANCHE

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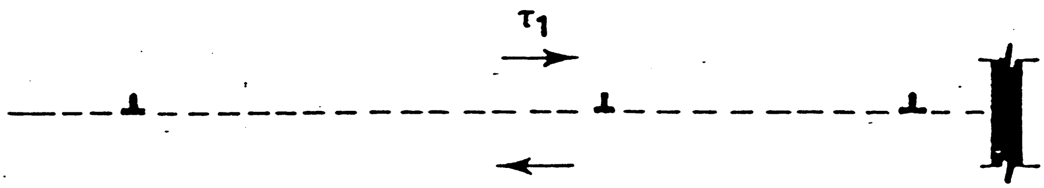
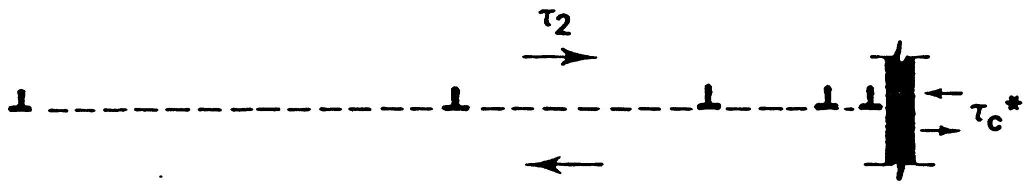
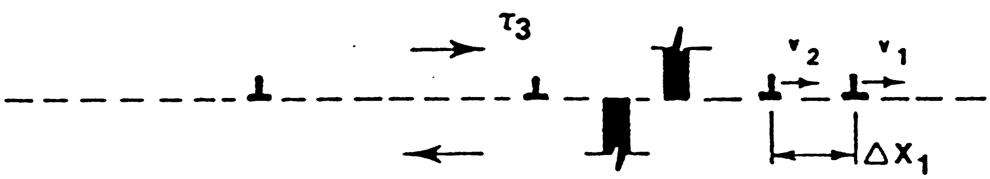
Naval Surface Weapons Center, Silver Spring, MD 20910, U.S.A.



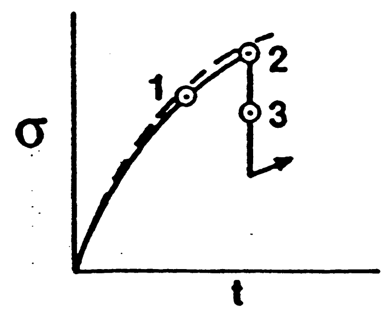
(a) isothermal stress build-up: n_1 dislocations



(b) critical stress concentration: $n_2\,\tau_2 = \tau_c^*$



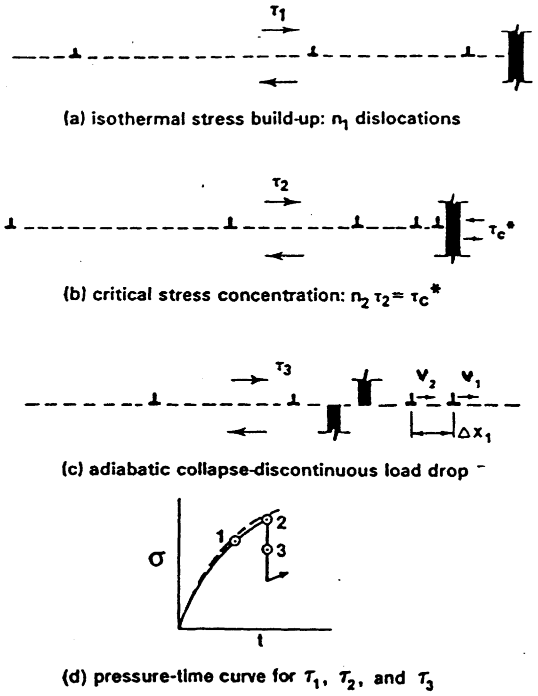
(c) adiabatic collapse-discontinuous load drop



(d) pressure-time curve for τ_1, τ_2, and τ_3

MODEL OF PILE-UP BREAKTHROUGH

Temperature Rise at a Dislocation Pile-up Breakthrough



(a) isothermal stress build-up: n_1 dislocations

(b) critical stress concentration: $n_2 \tau_2 = \tau_c^*$

(c) adiabatic collapse-discontinuous load drop

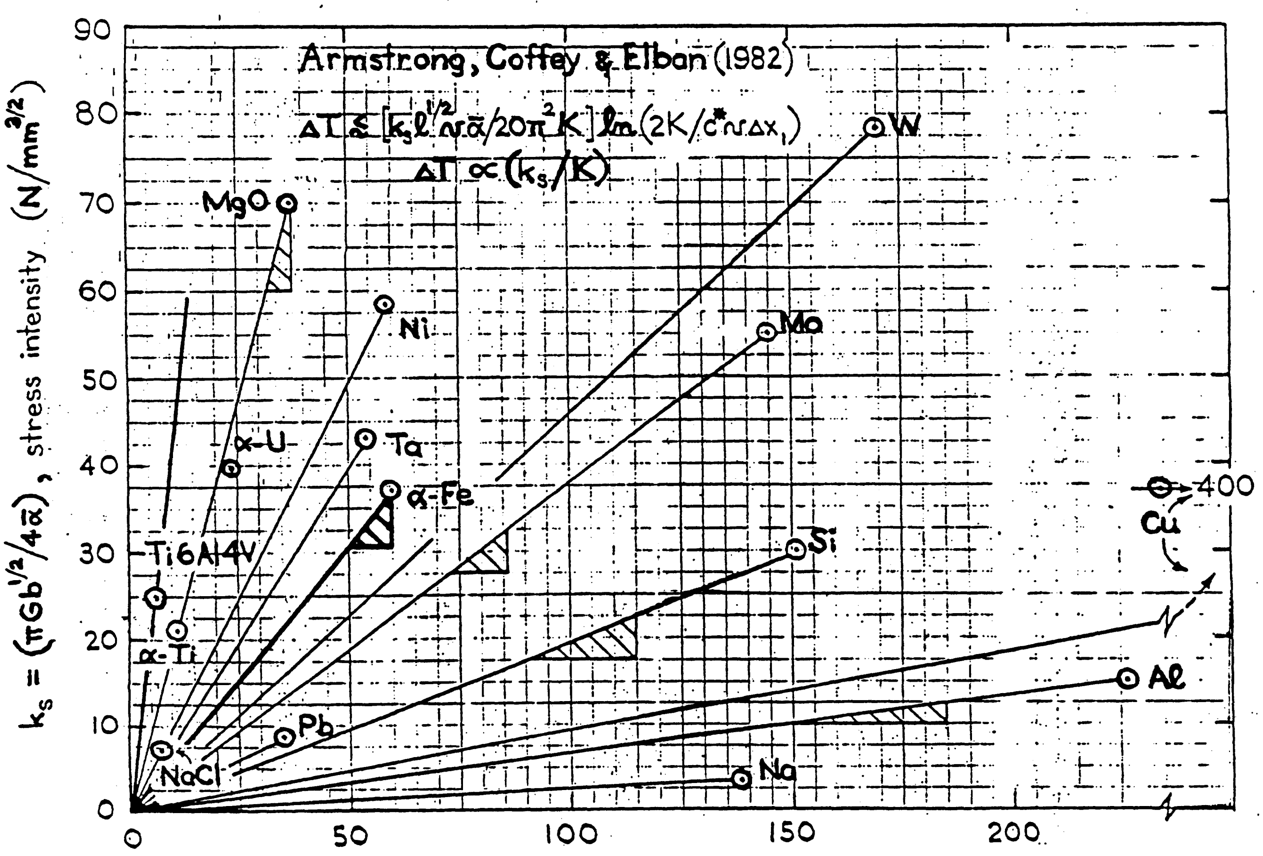
(d) pressure-time curve for τ_1, τ_2, and τ_3

MODEL OF PILE-UP BREAKTHROUGH

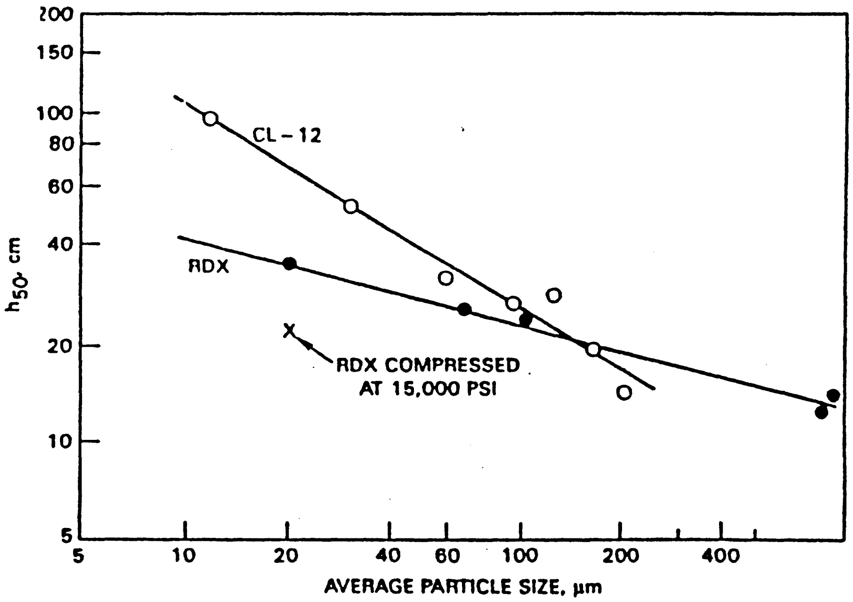
An upper limiting temperature rise, ΔT, is produced very locally by mechanical deformation confined to a single slip plane containing a blocking obstacle if release of the consequent dislocation pile-up is prevented until catastrophic failure occurs by cracking. Then,

$$\Delta T \leq \left[k_s \ell^{1/2} v\bar{\alpha}/20\pi^2 K\right] \ln\left(2K/c^* v \Delta x_1\right)$$

where k_s is the microstructural shear stress intensity for cracking, ℓ is the pile-up length, v is the released dislocation velocity, $\bar{\alpha} = 2(1-\nu)/(2-\nu)$ with ν being Poisson's ratio, K is thermal conductivity, c^* is specific heat per unit volume, and Δx_1 is the compressed spacing of dislocations at the pile-up tip. The sensitive material parameters are k_s and K, so ΔT is proportional to the ratio (k_s/K) as indicated graphically by various "slope" values.



IMPACT SENSITIVITY vs. PARTICLE SIZE FOR RDX AND OCTANITROBENZIDINE (CL-12)

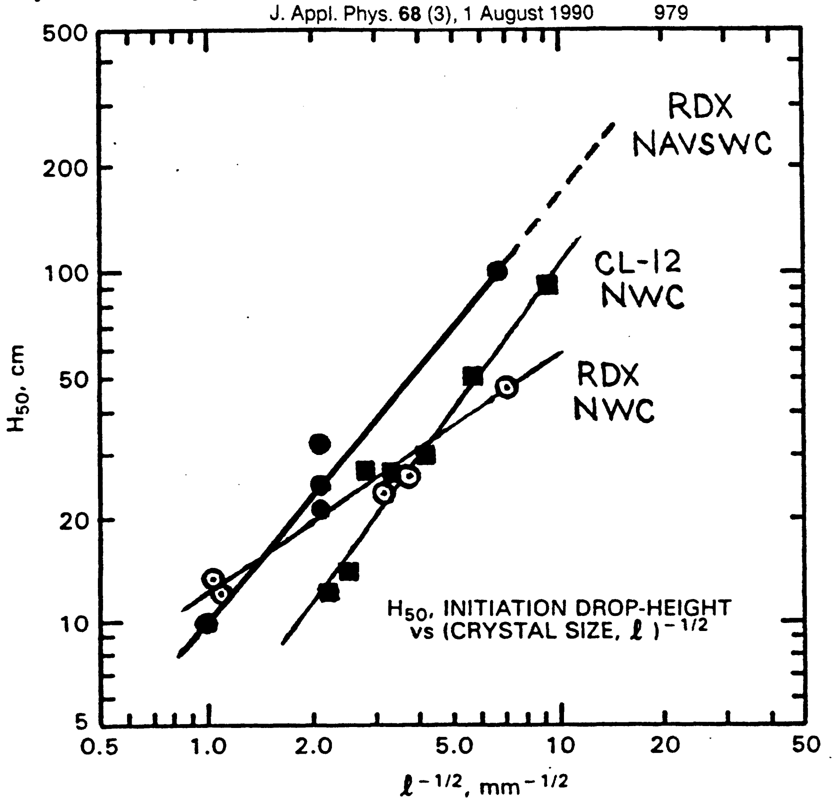


A.T. NIELSEN, Working Group Meeting on Sensitivity of Explosives, CETR, New Mexico Tech, 1987, pp. 256-276.

Crystal size dependence for impact initiation of cyclotrimethylenetrinitramine explosive

R. W. Armstrong
C. S. Coffey and V. F. DeVost
W. L. Elban

J. Appl. Phys. **68** (3), 1 August 1990 979



RDX : $(CH_2 \cdot N \cdot NO_2)_3$

CL-12 : $(NH_2C_6[NO_2]_4)_2$