



Center for Energetic Concepts Development

CONSEQUENT DISLOCATION MECHANICS FOR HOT SPOTS IN IMPACTED ENERGETICS*

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TOPICS

1. Dislocations in energetic crystals
2. Hardness aspects of elastic, plastic, and cracking behaviors
3. Dislocation mechanics
 - (i) The pile-up avalanche model
 - (ii) Crystal size predictions
4. Particle compaction and combustion
5. Shock results



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Dislocations in energetic crystals

| Material | Dislocation Strain Energy Coefficient ($E_{\perp/p}$), J | $\left(\frac{E_{\perp/p}}{\Delta H_{f/m}}\right)$ | Peierls-Nabarro Stress, (τ_p) , N/mm ² | $\left(\frac{\tau_p}{G}\right)$ | Dislocation Stress Intensity (k_s), N/mm ^{3/2} | $\left(\frac{k_s}{G}\right)$, mm ^{1/2} | $\left(\frac{\gamma}{Gb}\right)^{1/2}$ |
|----------|--|---|--|---------------------------------|---|--|--|
| RDX | 6.3×10^{-19} | 12 | 580 | 0.077 | 7.7 | 10×10^{-4} | 0.066 |
| PETN | 3.3×10^{-19} | 4.0 | 394 | 0.073 | 5.9 | 11×10^{-4} | 0.070 |
| AP | 1.2×10^{-19} | — | 1200 | 0.162 | 6.3 | 8.5×10^{-4} | 0.088 |
| LiF | 0.9×10^{-19} | 2.1 | 3100 | 0.050 | 29 | 4.6×10^{-4} | 0.14 |
| MgO | 2.4×10^{-19} | 1.9 | 8000 | 0.054 | 70 | 4.7×10^{-4} | 0.17 |

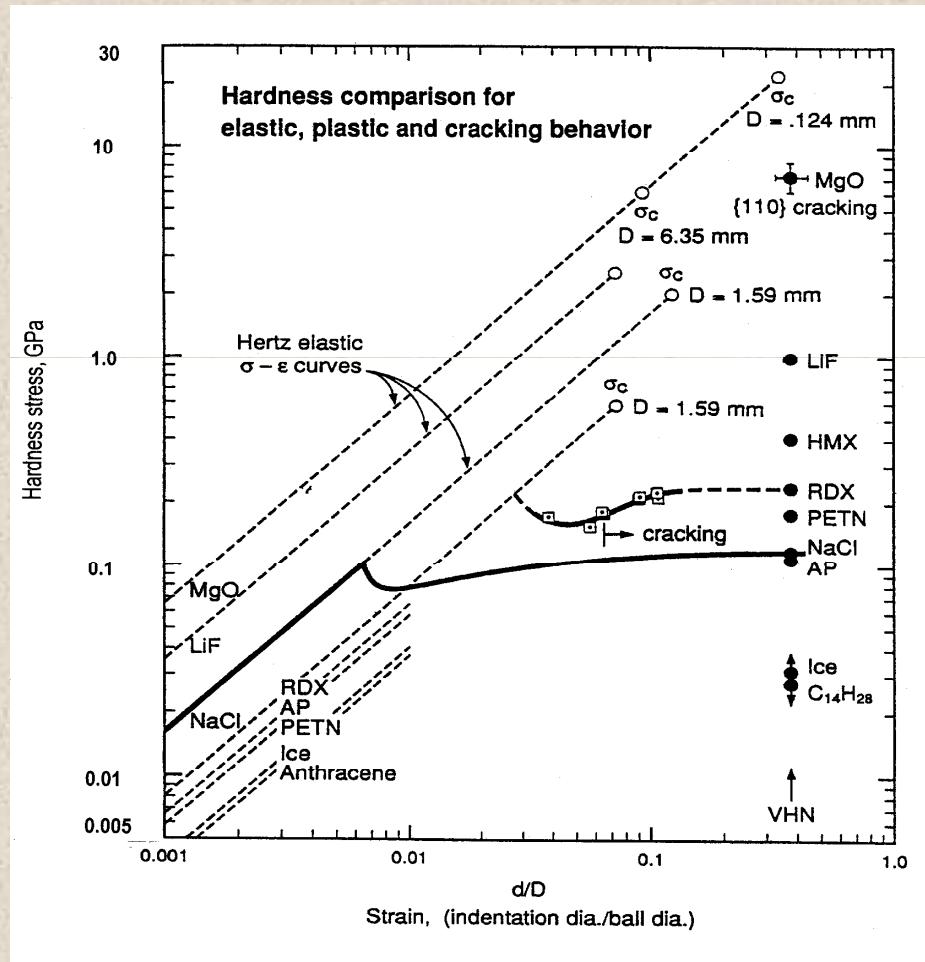
$$E_{\perp/p} = (Gb^2 \Delta \xi / 4\pi \bar{\alpha})$$

$$\tau_p (= \tau_{p,N}) = [2G/(1-\nu)] \exp [-2\pi d/(1-\nu)b]$$

$$k_s = (\pi G b^{1/2} / 4 \bar{\alpha})$$

R.W. Armstrong and W.L. Elban, in *Dislocations in Solids*, F.R.N. Nabarro and J.P. Hirth, eds., (Pergamon Press, Oxford, 2004), 12, pp. 403-446

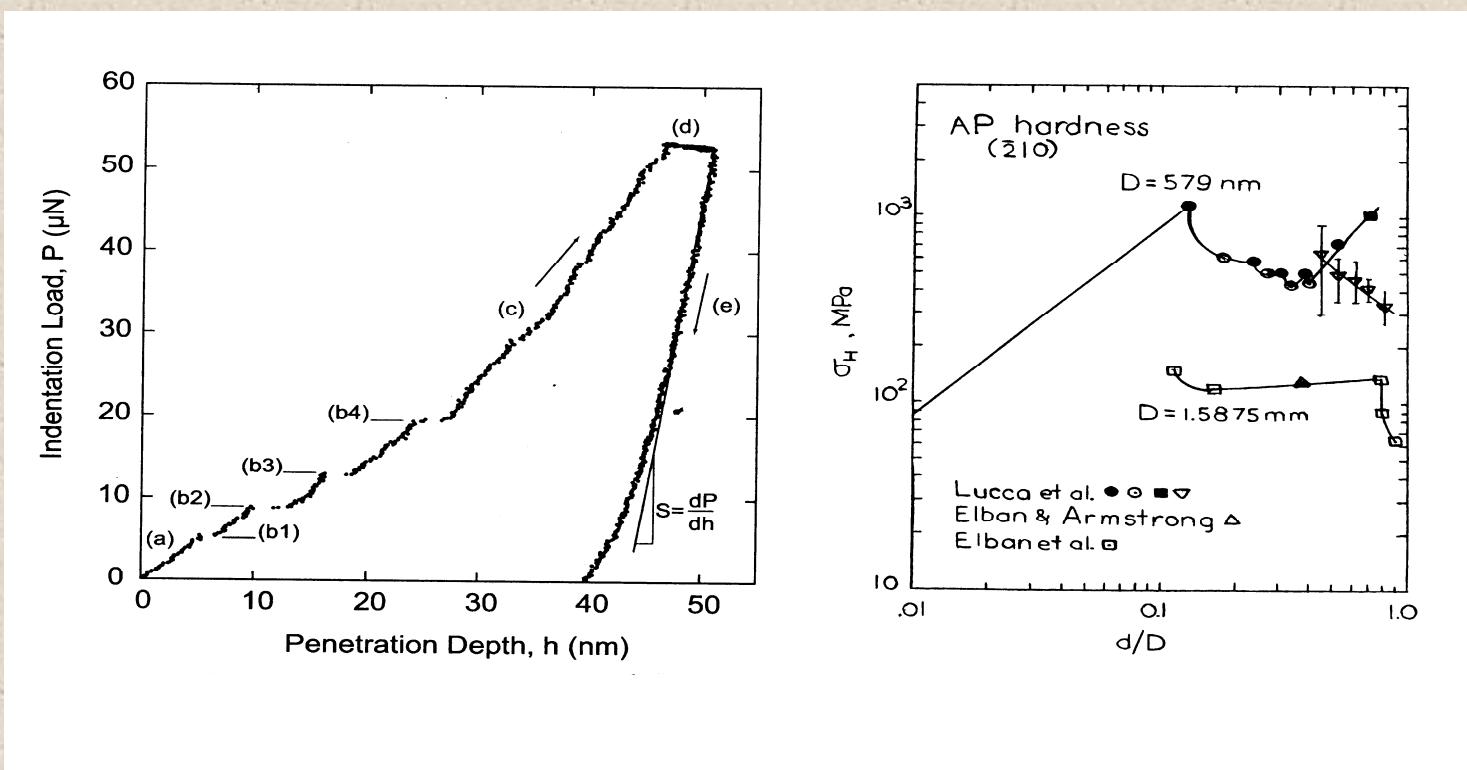
Hardness stress-strain description



R.W. Armstrong and W.L. Elban, Mater. Sci. Tech. 22, [4], 381-395 (2006)



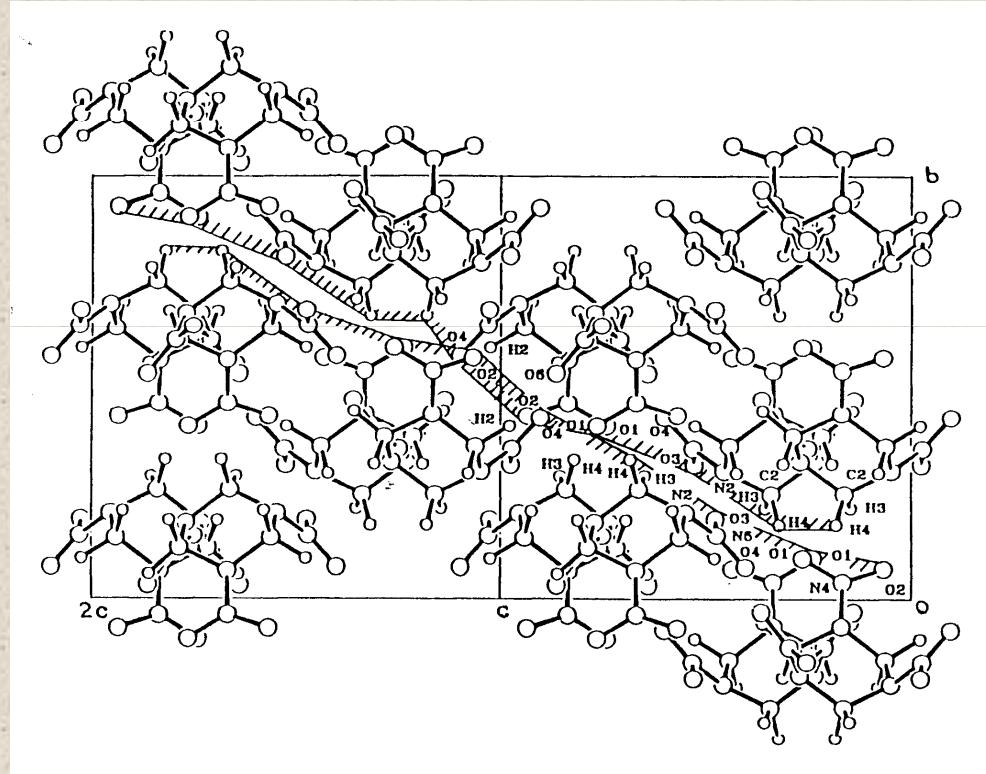
Nano- and macro-indentation stress - strain curves for AP



after D.A. Lucca, M.J. Klopfstein, O.R. Mejia, L. Rossettini, and L.T. DeLuca,
Mater. Sci. Tech. 22, 396-401 (2006).



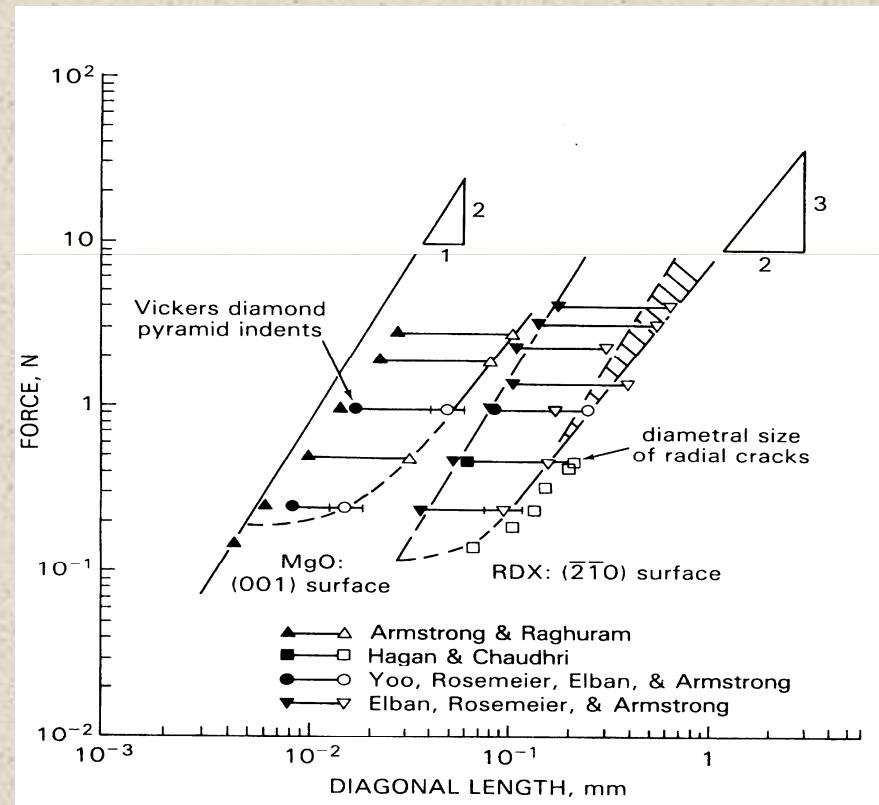
A reduced dislocation mobility



R.W. Armstrong, H.L. Ammon, Z.Y. Du, W.L. Elban and X.J. Zhang, in Structure and Properties of Energetic Materials, D.H. Liebenberg, R.W. Armstrong and J.J. Gilman, eds. (Mater. Res. Soc., Pittsburgh, PA, 1993) 296, pp. 227-232.



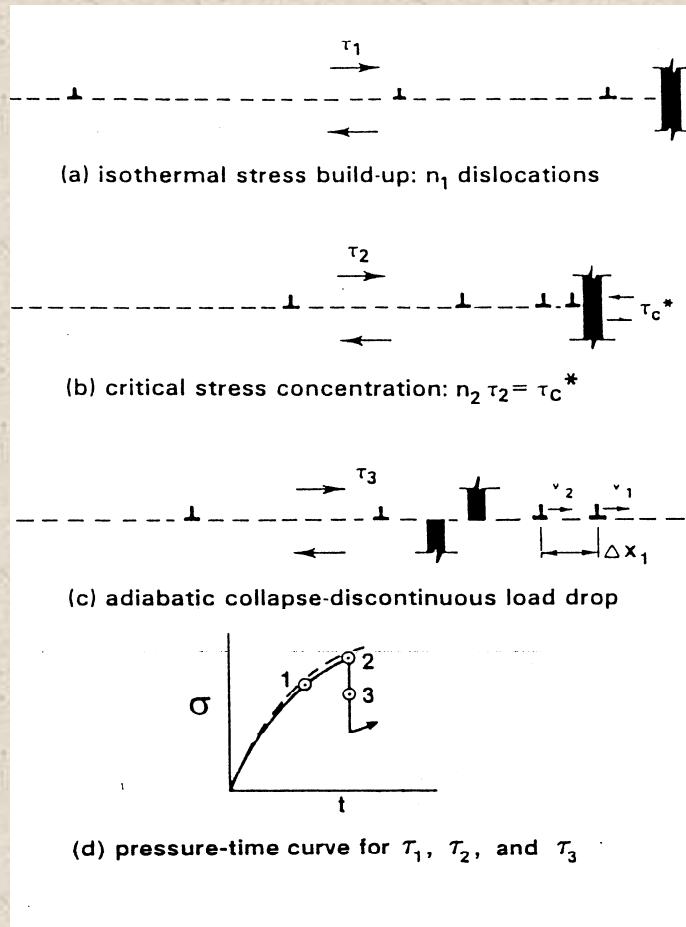
Comparative hardness and cracking results for MgO and RDX crystals



R.W. Armstrong and W.L. Elban, Mater. Sci. Tech., **22**, [4], 381-395 (2006)



Hot spot via the pile-up avalanche model



$$\Delta T \leq \frac{k_s l^{1/2}}{16\pi} \left(\frac{2v}{c^* b K} \right)^{1/2} \quad \text{if } \left(\frac{2K}{c^* v b} \right) \leq 1.0$$

$$\dot{\gamma} = Nbv,$$

$$v = v_0 \exp \left[- \left(G_0 - \int_{\tau_{th}^0}^{\tau_{th}} bA * d\tau_{th} \right) / kT \right],$$

$$bA * = W_0 / \tau_{th},$$

$$\tau_{th} \propto H_{50}^{1/n},$$

$$v = v_0 (H_{50}/H_{50}^0)^{W_0/nkT} \exp(-G_0/kT)$$

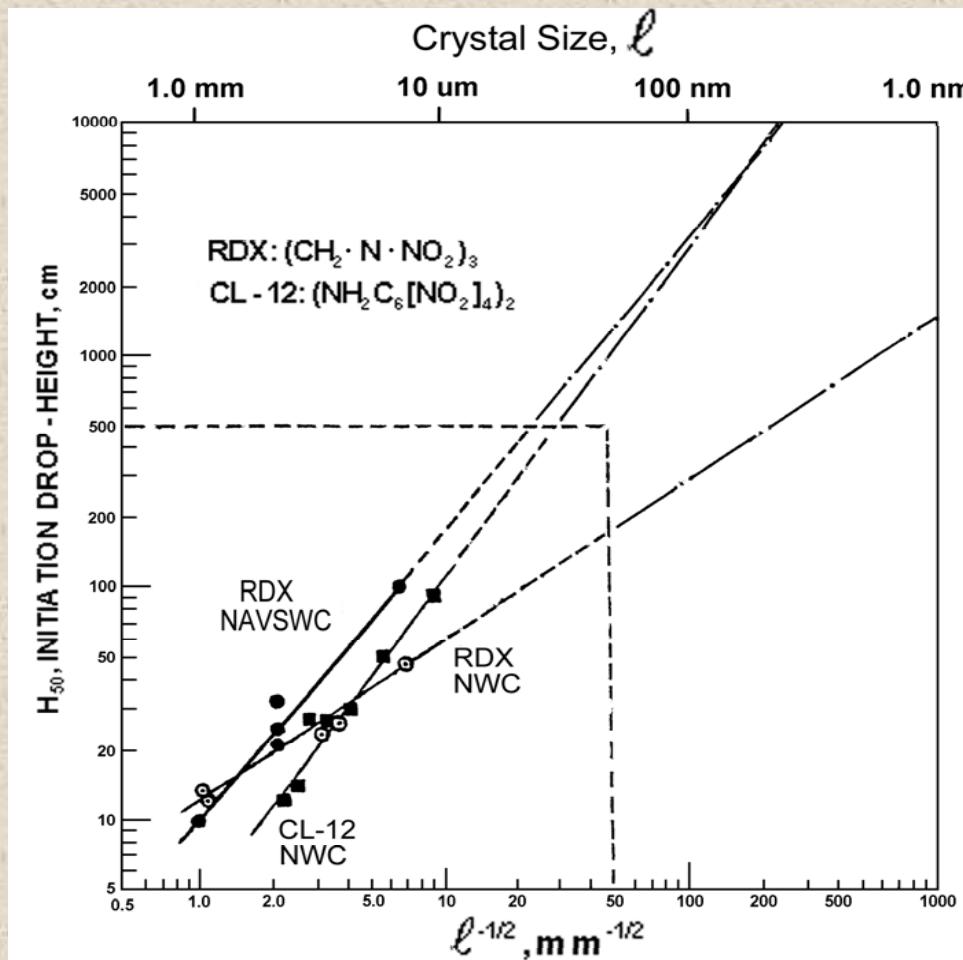
$$\begin{aligned} \log H_{50} &= \log H_{50}^* + (n/m^*) \log \{ [8\pi\sqrt{2}\Delta T \\ &\times K^{1/2} c^{*1/2} b^{1/2} / k_s v_0^{1/2} \\ &\times \exp(-G_0/2kT)] l^{-1/2} \}. \end{aligned}$$

$$m^* = W_0 / 2kT$$

R.W. Armstrong, C.S. Coffey, V.F. DeVost and W.L. Elban, J. Appl. Phys., 68, 979-984 (1990)



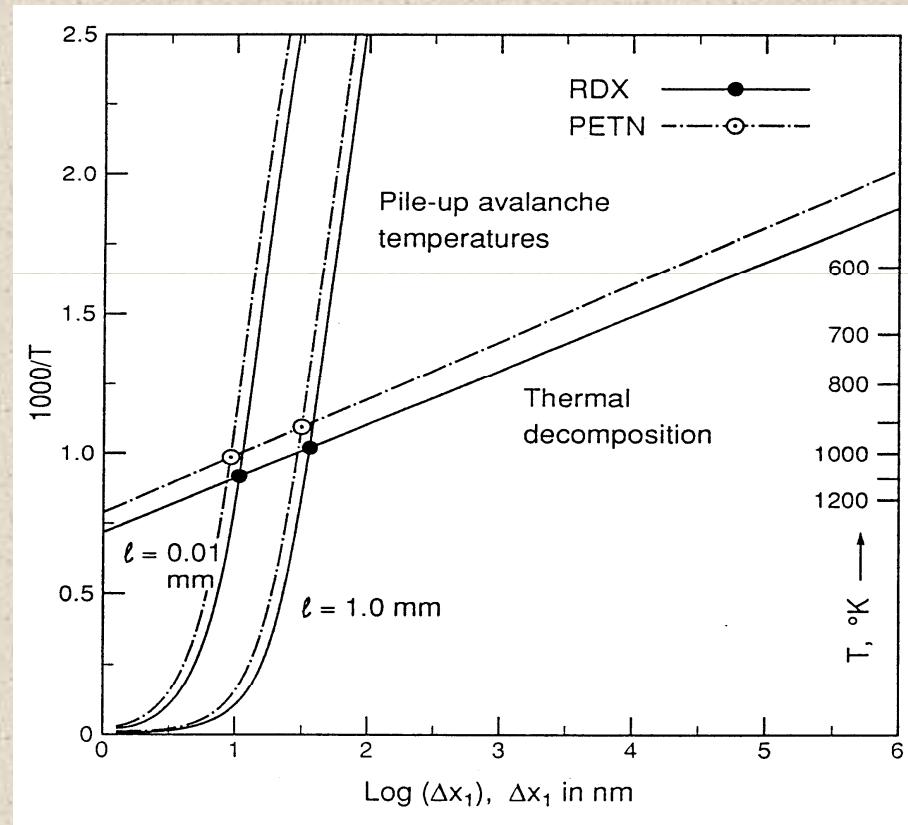
Drop-weight impact sensitivities



R.W. Armstrong, Rev. Adv. Mater. Sci., 19, 13-40 (2009)



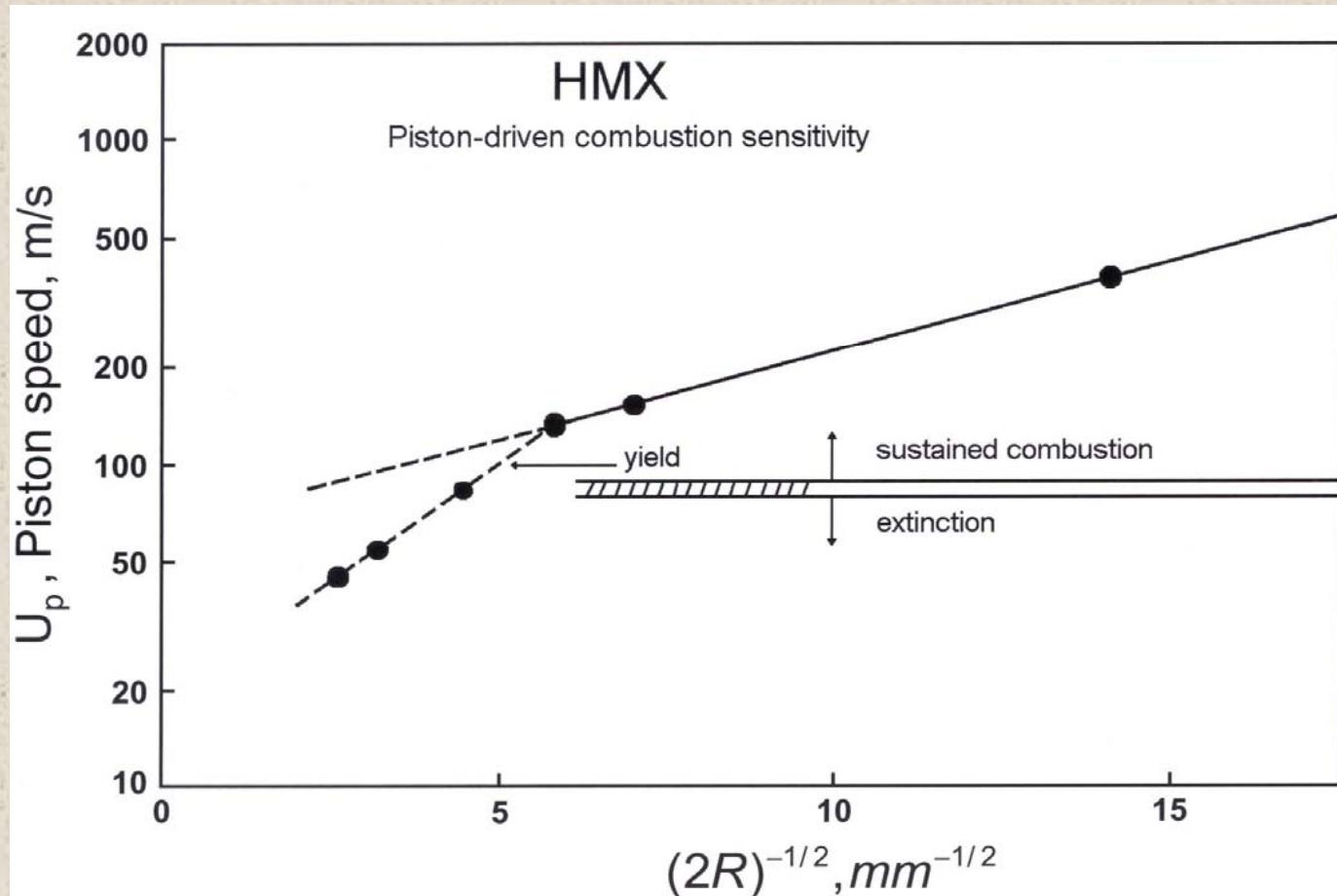
Pile-up avalanche and thermal decomposition temperatures for RDX and PETN



R.W. Armstrong, C.S. Coffey, V.F. DeVost, J. Appl. Phys. **68**, 979-984 (1990)



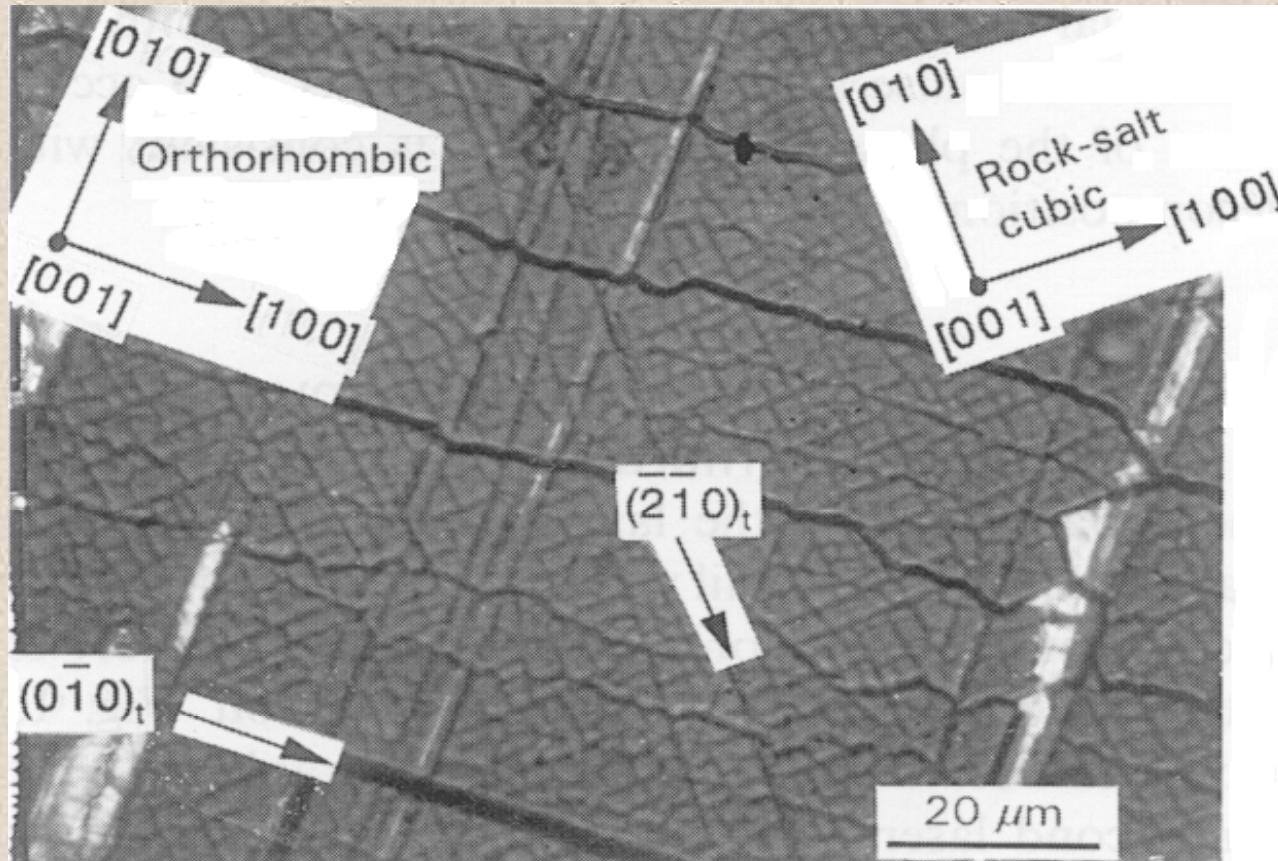
Combustion sensitivity dependence on crystal size



R.W. Armstrong, after K.A. Gonthier, J. Appl. Phys., **95**, 3482ff (2004).



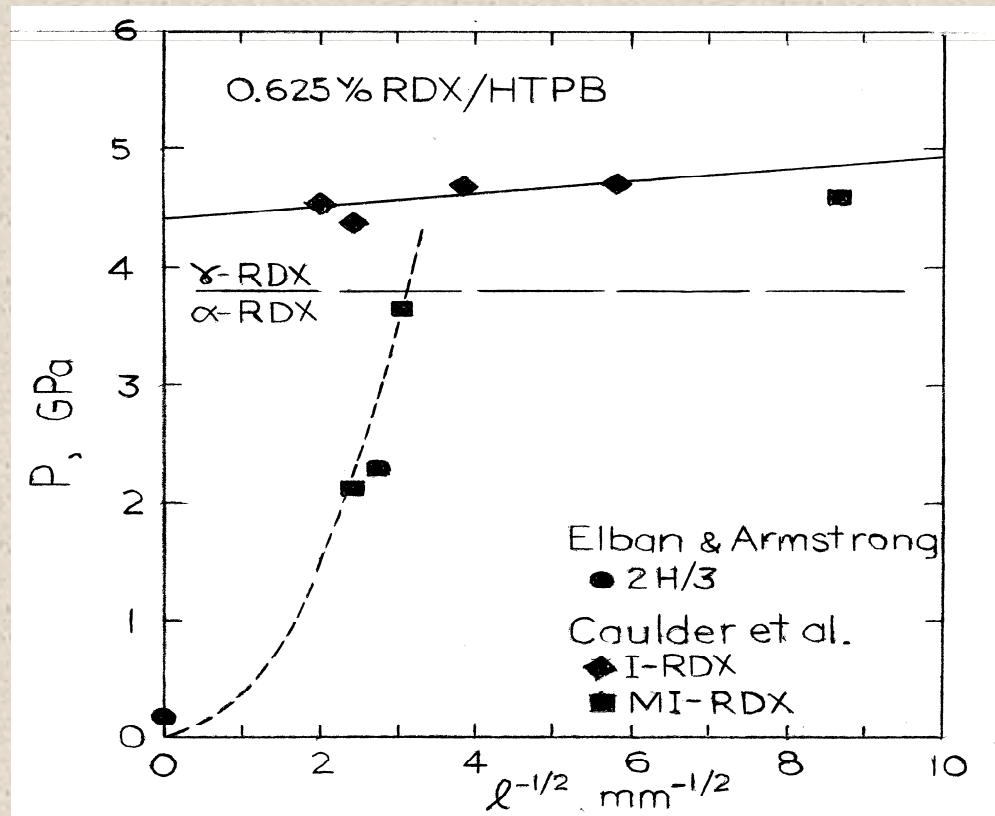
Cracking in laser-shocked AP crystal phases



A.L. Ramaswamy, H. Shin, R.W. Armstrong, C.H. Lee, and J. Sharma, J. Mater. Sci. 31, 6035ff (1996)



Shock sensitivity dependence on PBX crystal size



after S.M. Caulder, P.J. Miller, K.D. Gibson, and J.M. Kelly, Proceedings of the 13th Intern. Det. Symp., pp. 656-661, Norfolk, VA, July 2006



SUMMARY

1. Energetic crystal dislocations have very large self-energies and the brittleness and hot spot consequences are greater than for conventional metal or ceramic crystals.
2. A hardness-based stress – strain method of assessing energetic and related inert crystal elastic, plastic, and cracking behaviors illustrates the special energetic dislocation characteristics
3. Most important is prediction of a consequent crystal size dependence that is demonstrated for drop-weight impact, particle compaction, and shock sensitivity measurements.
4. Another consequence relates to understanding that shock-induced sensitivity measurements are made at relatively higher pressures than required for solid-state phase transformations.