HOT SPOTS FROM DISLOCATION PILE-UP AVALANCHES*

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Abstract. The model of localized adiabatic heating associated with release of a dislocation pile-up avalanche is described and re-evaluated. The model supplies a fundamental explanation of shear banding behavior in metal and non-metal systems. Now, a dislocation dynamics description is provided for more realistic assessment of the hot spot heating. Such localized heating effect was over-estimated in the earlier work, in part, to show the dramatic enhancement of the work rate, and corresponding temperature build-up, potentially occurring in the initial pile-up release, say, at achievement of the critical dislocation mechanics-based stress intensity for cleavage. Proposed applications are to potentially brittle metal, ionic, and energetic material systems.

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INTRODUCTION

The dislocation pile-up model is shown in Fig. 1.

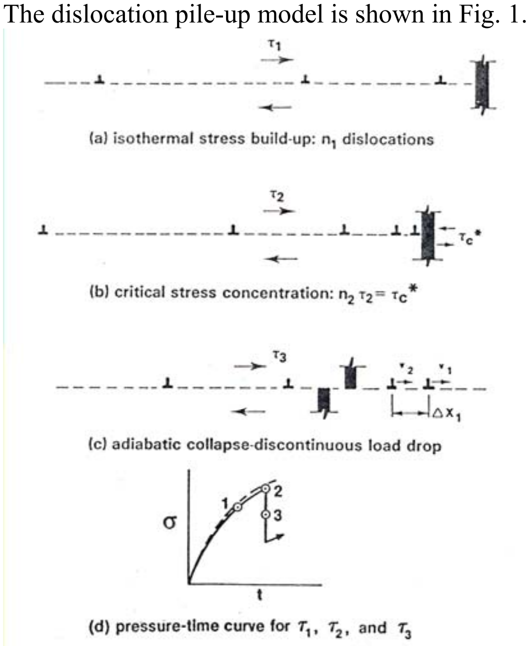

FIGURE 1. Stages of dislocation pile-up release [1].

AVALANCHE CHARACTERISTICS

Two important aspects of the avalanche-assisted enhancement of the local material plastic work rate are derived from the critical condition:

$$n(\tau_a - \tau_o) = \tau_c^*$$

for which n is the number of (free) pile-up dislocations, τ_a is the applied shear component of stress, τ_o is the lattice friction stress resisting individual dislocation movement, and τ_c^* is the critical component of shear stress. First, substitution of the linear dependence of n on effective stress and slip diameter gives a microstructural stress intensity, k_s, evaluated at the (highest) crack nucleation limit as $\pi G b^{1/2}/4\alpha$, where G is the shear modulus, b the dislocation Burgers vector and $\alpha = 2(1-\nu)/(2-\nu)$, with ν being Poisson's ratio [2]. Thus, n has its largest value at this τ_c^*. Secondly, at sudden pile-up release, the first now free dislocation is driven by the effective stress, $(n-1)(\tau_a - \tau_o)$, and the one behind by $(n-2)(\tau_a - \tau_0)$, and so on [2]. The combined result is an appreciably enhanced work rate with greatest potential temperature rise.

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The temperature rises for such dislocation avalanches were over-estimated by the relations

$$\Delta T \leq [k_s \ell^{1/2} v/16\pi K] \ln [2K/c^* vb]$$

or

$$\Delta T > [k_s \ell^{1/2}/16\pi] [2v/c^* bK]^{1/2}$$

dependent on whether $[2K/c^* vb] > 1.0$, or < 1.0, respectively [1]. The material constants for metals and ionic solids fit the first condition and those for molecular energetic materials fit the second condition. Substitution of a thermally-activated dislocation velocity for v

$$v = v_o \exp[-(G_o - \int bA \, d\tau_{th})/kT]$$

led [3], then, with $A = W_o/b\tau_{th}$ and τ_{th} proportional to an exponential dependence on the drop-weight height for 50% probability of initiation, H_{50}, to prediction of a log-log relationship for H_{50} versus $\ell^{-1/2}$.

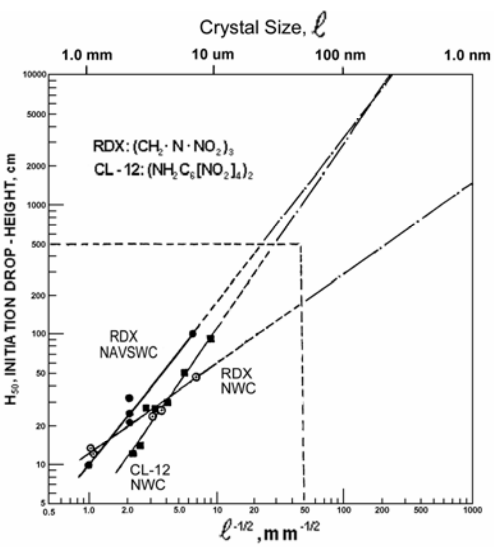

FIGURE 2. H_{50} vs $\ell^{-1/2}$ for impacted crystals.

In the equation for v, G_o is the Gibbs free energy for dislocation activation in the absence of a thermal component of stress, τ_{th}, A is dislocation activation area, and k is Boltzmann's constant. Figure 2 gives reasonable confirmation of the predicted behavior measured for RDX, ($[CH_2 \ N \ NO_2]_3$), and CL-12, ($[NH_2 C_6 \{NO_2\}_4]_2$).

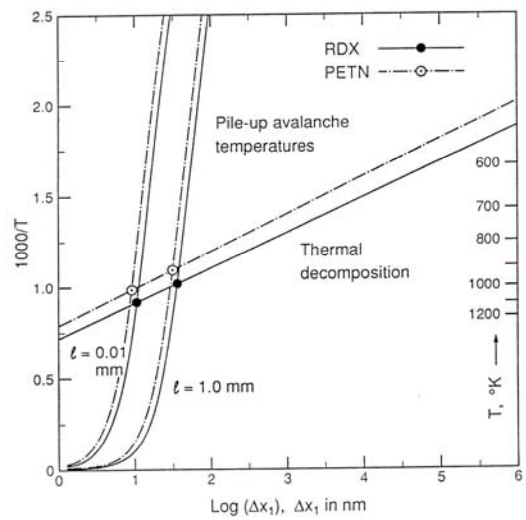

FIGURE 3. Pile-up and explosion temperatures.

The pile-up predictions have been compared with thermal explosion predictions for RDX and PETN, ($C[CH_2 OH]_4$) [3,4].

In Figure 3, the thermal explosion temperatures themselves follow an Arrhenius law that carries through the analysis to give a reciprocal dependence of the critical temperature on the logarithm of the hot spot size, Δx_1. The pile-up temperatures are shown for two crystal sizes that may be seen from the comparison of curve-and-line intersections to give a higher required temperature for initiation of thermal decomposition for smaller crystal sizes [4]. Furthermore, the easier initiation of PETN compared to RDX, at the same crystal sizes, is seen to occur because of the lower thermal explosion temperature for PETN, that is interpreted to result because of the lesser stability of the PETN molecule compared to RDX.

The relative brittleness of RDX and related crystal structures may be assessed in one way in terms of a cleavage susceptibility index $(\gamma/Gb)^{1/2} = 0.066$ for RDX [5] and 0.070 for PETN; values < 0.29 are indicative of brittleness in metals. The index compares the ease of cracking with the difficulty of generating dislocations. A further comparative elastic/plastic/cracking basis for assessing the relationship of plastic flow to cracking is shown below on an indentation hardness stress-strain basis [6] in Figure 4.

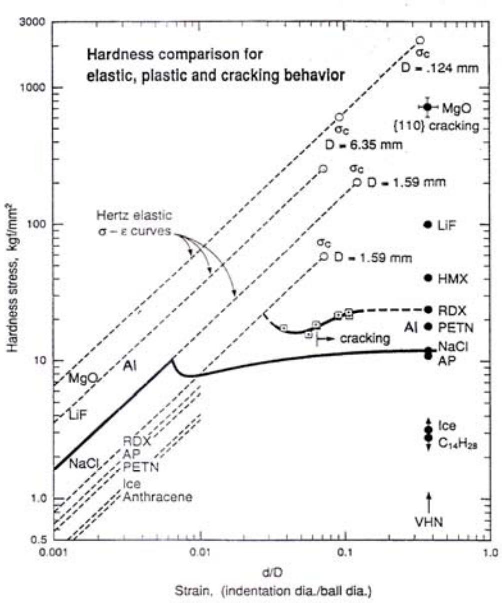

FIGURE 4. Elastic/plastic/cracking hardnesses.

In the Figure, with Al recently added [7], the hardness stress is the equivalent mean pressure on a (steel) ball indenter and the effective strain is the contact diameter, d, divided by the ball diameter, D. Vickers (diamond pyramid) hardness numbers, VHN, are plotted at (d/D) = 0.375. The elastic unloading doesn't alter d for a plastic indentation. The main point here, however, is to note that the hardness stress for RDX is ~3 times lower than the hardness stress needed elastically, σ_c, for cracking at the same ball size. The ratio of hardness stresses provides an estimate of the number of dislocations needed plastically to reach the cracking stress.

The new consideration then is the extent to which the analytic dislocation pile-up equations for dislocation number, pile-up length, and effective shear stress might be applicable at small dislocation numbers. Such comparison has been made for various types of pile-up configurations [8] and the perhaps surprising result of applicability at small numbers leads to the possibility of illustrating the proposed avalanching effect in a numerical model of such a breakthrough.

A pioneering numerical model description of pile-up release dynamics was given by Gerstle and Dvorak [9] for the hypothesized case of a relatively weak obstacle and employing small dislocation numbers. In the model, the obstacle resistance of a grain boundary was represented by a narrow region requiring a higher viscosity than the grain interior. Thus, the piled-up dislocations at the single-ended slip band tip were held up until forced through the boundary region by others following behind. An exponential dependence of the dislocation velocity on the effective shear stress was employed with constants fitted to the grain size dependent yielding of steel. Figure 5 provides an example result for a pile-up of 17 dislocations in which x_j is the position of the j'th dislocation counted from the lead position and (t/t_y) is the relative time scale determined by the time for the lead dislocation to pass through the obstacle. In the Figure, the dashed "s" curve is the average positional movement for all of the dislocations.

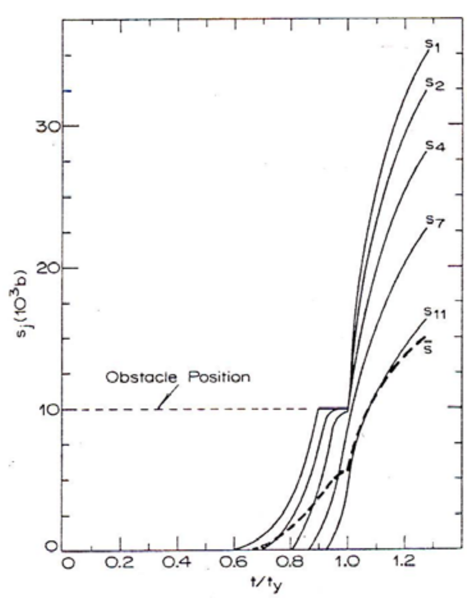

Figure 5. Dislocation pile-up releases [9].

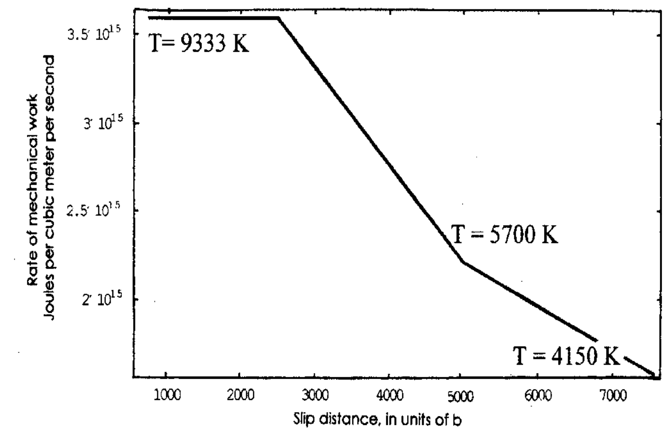

Figure 6. Plastic work rate and temperature rise for a modeled dislocation avalanche in iron [11].

Attention is directed in Figure 5 to the speed at which the lead dislocations are released. Even for this case of a release (obstacle) stress only just greater than 3 times the effective applied stress, the lead dislocation is seen to move initially at greater than 100 times the average dislocation velocity leading up to the obstacle.

Taylor and Quinney [10] are generally credited with the experimental observation, made at large material straining, that most of the plastic work goes into heating the deformed material. In the present case modeled after Gerstle and Dvorak and without loss or creation of additional dislocations in a slip length, ℓ, containing sixteen dislocations, the work rate, that is assumed to be confined within the slip band thickness for the released dislocations, is expressed [11] as

$$W = \sum \tau_{i,eff} \cdot \gamma_i = (C/\beta)\Delta T$$
$$\partial W/\partial t = (C/\beta)\partial(\Delta T)/\partial t$$
$$= (1/\ell)\sum \tau_{i,eff}\, v_i$$
$$\Rightarrow \Delta T \approx (\beta/C)\cdot(1/\ell)\sum \tau_{i,eff}\, v_i\, \Delta t_i$$

β is the fraction of plastic work converted to heat, and C is the specific heat and the sum is over all dislocations and the effective stresses are evaluated at each i'th dislocation with its corresponding velocity at the time t_i. Figure 6 shows evaluation of the work rate achieved over micron distances. The temperatures at each position are computed for the total conversion of the plastic work. Though still relatively high, the temperatures are lower than those previously overestimated for pile-up release at cracking [2] and, for which, the dislocation shear wave speed, more than 100 times greater than for the lead dislocation here, had been employed for the released dislocation velocities.

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