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Investigation of hot spot characteristics in energetic crystals

R.W. Armstrong[a,*], H.L. Ammon[b], W.L. Elban[c], D.H. Tsai[d]

[a]AFRL/MNME, 2306 Perimeter Road, Eglin AFB, FL 32542, USA
[b]Department of Chemistry and Biochemistry, University of Maryland, College Park, MD 20742, USA
[c]Loyola College, 4501 N Charles Street, Baltimore, MD 21210, USA
[d]10400 Lloyd Road, Potomac, MD 20854, USA

Abstract

The model hot spot characteristics of energetic crystals, particularly, of cyclotrimethylenetrinitramine (RDX) and related materials, are described within a molecule-to-crystal–lattice-to-dislocation defect framework, as developed under the guidance of R.S. Miller. The purpose was to trace the dimensional scale at which controlling influences occurred for energetic material responses to imposed mechanical forces and/or deformations. Important consequences of the work include: (1) explanation of a substantial energetic crystal lattice resistance to shear-type deformations; (2) molecular dynamics modeling demonstration of significant heating associated with defect relaxations; and (3) dislocation pile-up prediction of a greater drop-weight impact height requirement for initiation of smaller crystals. © 2002 Elsevier Science B.V. All rights reserved.

Keywords: RDX; Energetic crystals; Hot spot characteristics; Dislocation pile-ups; Molecular dynamics

1. Introduction

Richard (Dick) S. Miller reported mainly on the chemistry of new energetic molecules in the Materials Research Society Symposium: Decomposition, Combustion and Detonation Chemistry of Energetic Materials [1]. The symposium followed after an earlier materials science based one, at the same venue, on the Structure and Properties of Energetic Materials [2]. The total symposium articles for both meetings, contributed in part by investigators supported under Office of Naval Research Programs managed by Dick, give evidence of his organized approach in tracking the hierarchical levels at which explosive material properties, in general, and explosive decompositions, in particular, could be understood and as a building process towards development of predictive equations for describing the overall behaviors of this special class of materials.

In a number of workshops published by the Chemical Propulsion Information Agency, notably one in 1986 at Los Alamos National Laboratory [3], Dick brought together chemistry, physics, engineering, and materials science colleagues to make connections in the energetic materials subject area spanning picosecond to millisecond time scales and involving nanoscale to macroscale experiments and model calculations. Yuan T. Lee was informed at the LANL meeting of having won the Nobel Prize that year in chemistry. Fig. 1 shows examples, schematically, of the important discussion undertaken between investigators who were looking into different aspects of the decomposition properties of cyclotrimethylenetrinitramine (RDX) crystals encompassing: (a) proposed decomposition of colliding RDX molecules in molecular beams; (b) the difficulty of specific [1 0 0] (0 4 0)

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* Corresponding author.
E-mail address: ronald.armstrong2@eglin.af.mil (R.W. Armstrong).

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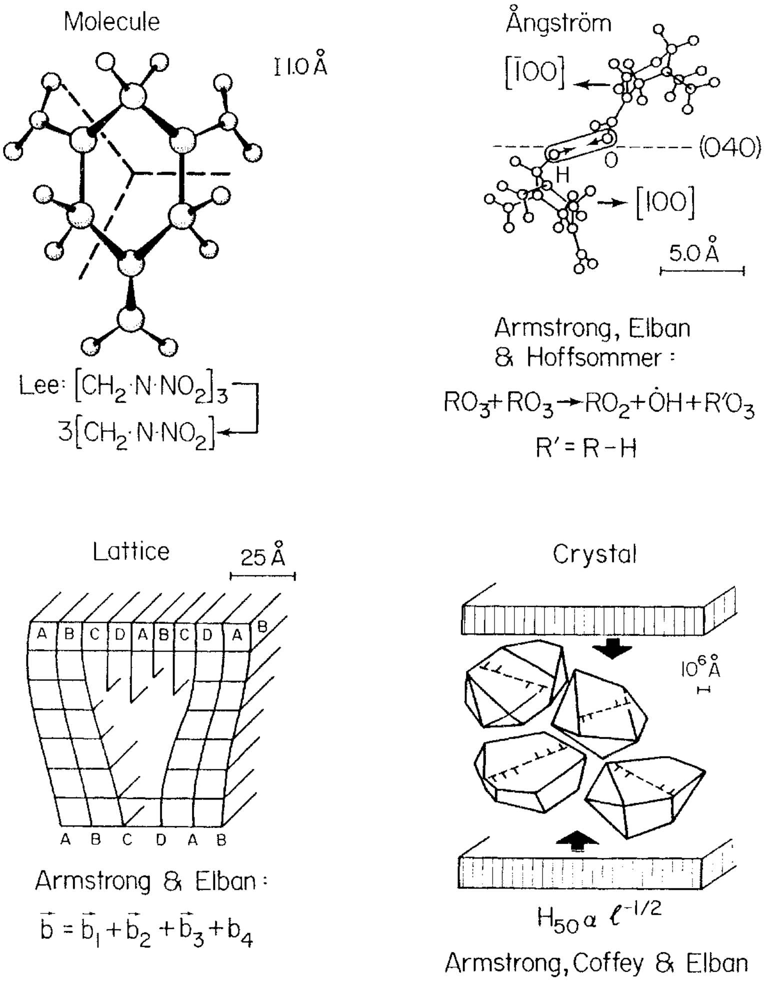
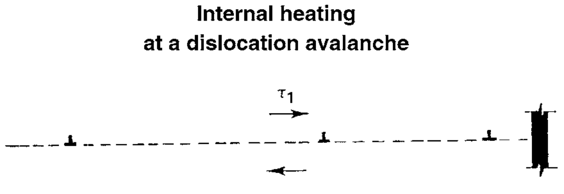


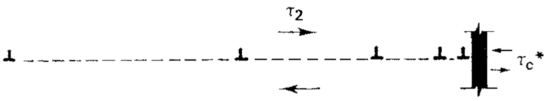
Fig. 1. Levels of modeling to characterize the decomposition properties of RDX.

shear deformation in the RDX lattice; (c) a theoretical partially dislocated structure in the RDX lattice; and (d) the multiplicative effect of dislocation pile-up avalanches in drop-weight impacted RDX crystals.

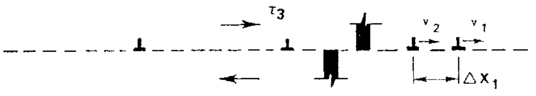
Follow-on collaborative workshops were organized in Europe on energetic material properties also [4,5]. In [5], a preliminary report was given of the internal defect structure of RDX crystals and influence of their external morphologies on shock sensitivity. Also, preliminary results were presented of upper limiting model calculations for hot spot temperatures and life times corresponding to dislocation pile-up avalanches being triggered by crystal cleavage. Fig. 2 shows schematic illustration of the model consideration of reasonably gradual (isothermal) stress build-up at a developing dislocation pile-up until breakthrough occurs to give essentially adiabatic dissipation of the pent-up dislocation interaction energy. The latter research result came from a joint ONR-supported activity at the University of Maryland and the Naval Surface Warfare Center, started first at the NSWC White Oak Laboratory and now continued at NSWC Indian Head Division. The consequent research effort on elucidation of hot spot development in energetic materials, undertaken by the current authors and other colleagues, is the focus of this paper dedicated to Dr. Richard Miller. Four topics are covered: (1) deformation/cracking at the crystal



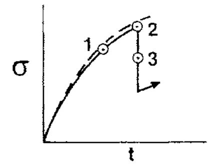
(a) isothermal stress build-up: n_1 dislocations



(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

Fig. 2. Schematic illustration of successive stages of dislocation pile-up formation and catastrophic collapse to provide adiabatic dissipation of the pent-up strain energy.

lattice level; (2) a comparative hardness stress–strain basis for assessing deformation and cracking; (3) molecular dynamics evaluation of hot spot requirements; and (4) the dislocation pile-up avalanche model for hot spots.

2. Results and discussion

2.1. Deformation/cracking of energetic crystals

Early dislocation etch pitting observations made at microindentation hardness impressions put into the exposed crystallographic {2 1 0} growth face of an RDX (cyclotrimethylenetrinitramine) crystal gave indication that dislocation generation and movements to create the residual indentations were difficult [6]. The dislocation etch pits in RDX were closely clustered in the immediate vicinity of the indentations, say as compared with the extended movement of dislocations in "rosette wings" spreading from indentations in LiF crystals. Thus, the indication was that RDX was behaving in a relatively hard manner despite the otherwise weak molecularly-bonded nature of the crystal lattice. In addition, cracking was observed to occur frequently at such indentation sites [7], thus giving further indication that the dislocation processes were occurring at stresses near to those required for crystal cleavage. The experimental observations were attributed to the fundamental difficulty of dislocation movement occurring by required shear-type displacements of individual molecules in the RDX orthorhombic Pbca lattice structure.

Fig. 3 shows, on the basis of the established RDX crystal lattice structure, an example of the mutual interference that occurs between adjacent molecular appendages when forced to undergo, albeit rigid ⟨1 0 0⟩ shear displacements (in and out of the {1 0 0} plane of the figure) across the observed {0 2 1} slip plane. In this case, attention is directed to the cross-hatched blockage between oxygen "02" and "04" positions of adjacent molecules that are shown midway along the ordinate *b* unit cell axis. Such blockages, normal to the observed {0 2 1} plane of shear, are not removed by the intrinsic partially sheared character of the dislocation self-strain field, as schematically illustrated in Fig. 1. These particular intermolecular interactions appear to be just those required to explain the occurrence of oxygen bond breakage leading to nitroso-compound formation, as detected in drop-weight impact test samples recovered after experiencing near initiation drop-weight heights [8]. The schematically modeled result is in agreement with expectation of a high crystal shear resistance and relates as well to a particular forced shear displacement potentially leading to an experimentally-determined chemical reaction pathway for further molecular decomposition. For example, Behrens and Bulusu [9] have reported nitroso-compound formation in pyrolysis experiments conducted under well-controlled temperatures and pressures.

Such modeling efforts at the crystal lattice scale were applied to the comparison of dislocation shear-associated slip mechanisms being favored in the RDX crystal lattice, albeit at relatively high stresses, versus

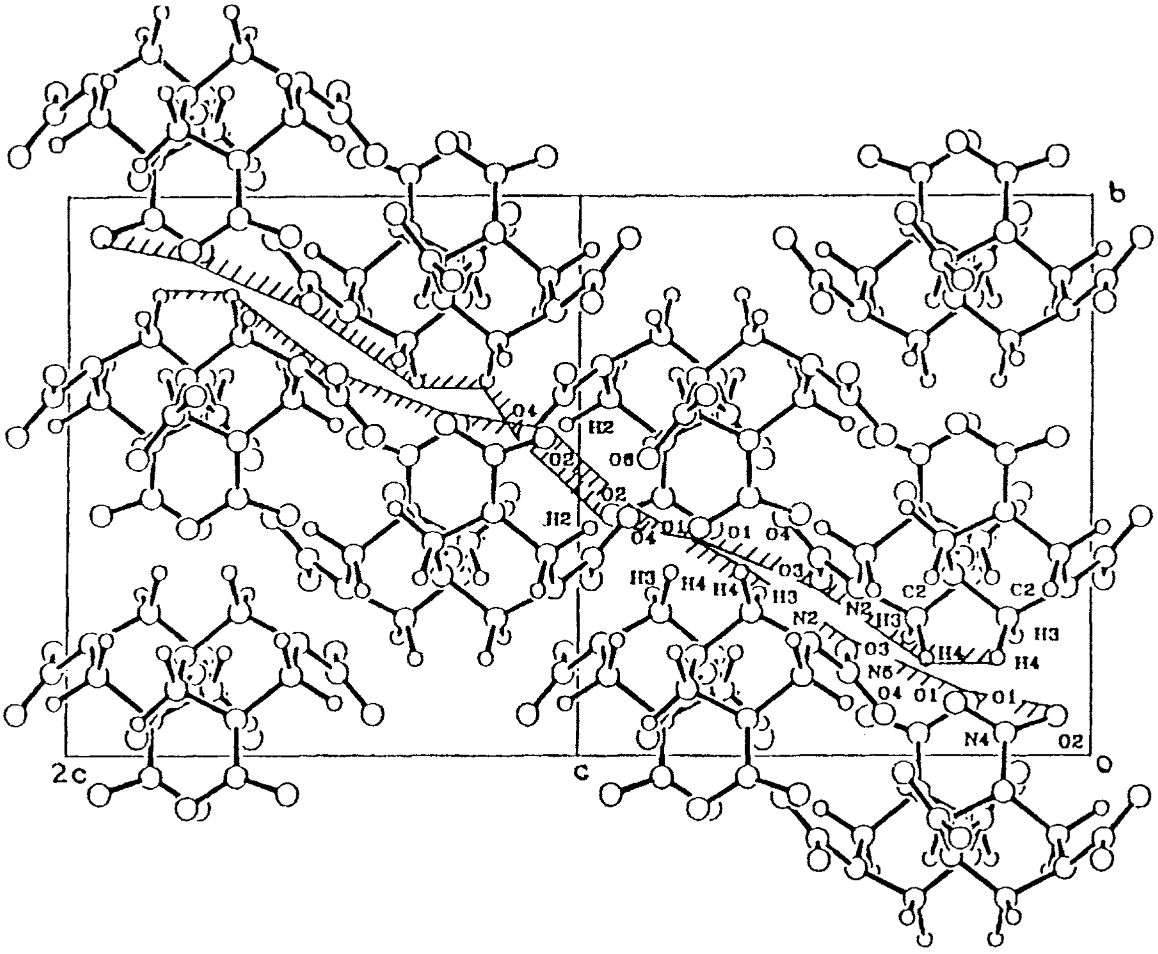


Fig. 3. Modeled molecular interactions in RDX obstructing ⟨1 0 0⟩ {0 2 1} slip.

deformation induced twinning-type reorientation of the crystal lattice being favored in the monoclinic *P21/n* crystal lattice of molecularly-related cyclotetramethylenetetranitramine (HMX) [10]. The greater flexibility of the HMX molecule was shown by model construction and activation energy estimates to allow a reasonable molecular displacement and flexural pathway to produce ⟨1 0 1⟩ {1 01} twinning.

2.2. Comparative deformation/cracking behaviors on a hardness stress–strain basis

The issue of whether energetic crystals such as RDX are truly relatively hard may be resolved in one way by comparing their indentation hardness stress–strain behaviors with those measured for other crystal structure types. One rather comprehensive method for doing this, particularly relating to a variety of hardness testing techniques, was demonstrated previously for hardness test results obtained quasi-statically at ambient temperatures for NaCl and MgO crystals. The method involves assessment of the combined elastic/plastic/cracking behavior of a material on a continuous indentation hardness stress–strain basis [11].

Fig. 4 provides an example of such computed and measured hardness results for a variety of energetic and inert crystals. The figure includes results to be described for RDX, HMX, pentaerythritol tetranitrate (PETN), and ammonium perchlorate (AP) crystals

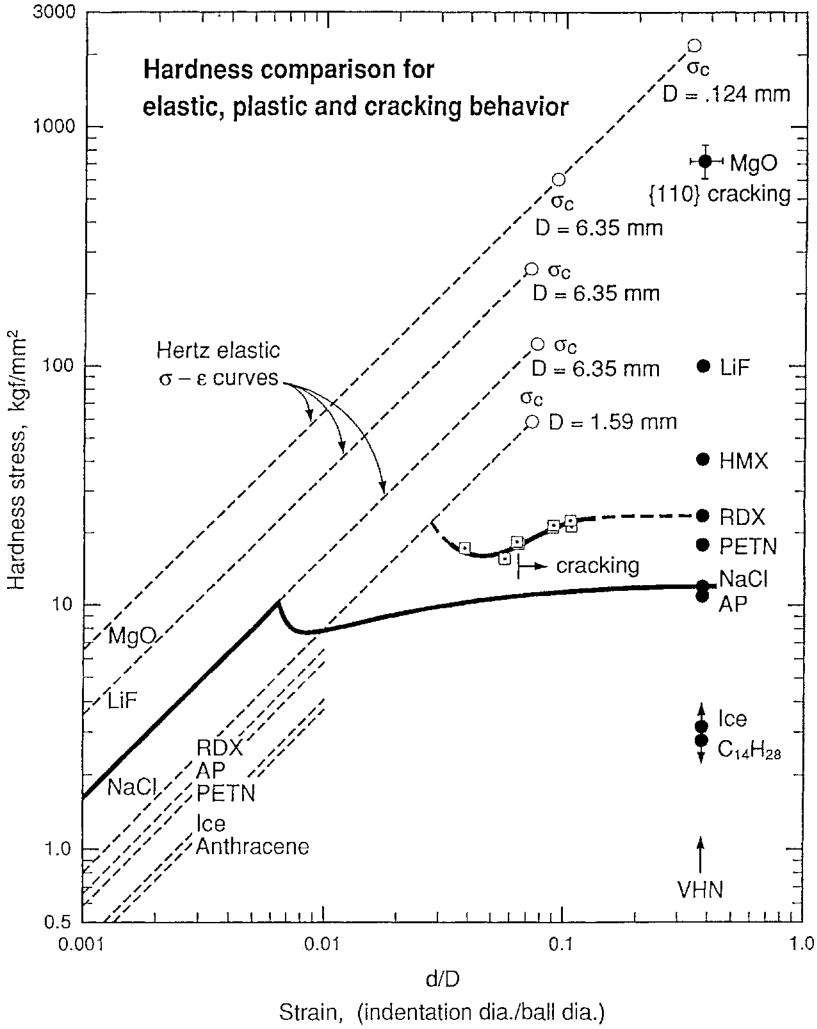


Fig. 4. Hardness stress–strain basis for elastic/plastic/cracking behaviors.

that may be usefully compared with other better-known crystal hardness properties, such as for MgO, LiF, NaCl, ice and anthracene crystals. The scatter of variously reported Vickers hardness number (VHN) measurements, made with a diamond pyramid indenter, are shown in the figure for MgO along with indication of higher hardness expectations for ice and lower, for anthracene. The figure makes connection, at lower applied contact stresses, between the predicted Hertzian elastic contact behaviors achieved with a ball indenter, and at larger imposed indentation strains, between the equivalent ball indentation stresses obtained from the VHN measurements, corresponding to a plastic contact stress based on the residual indentation size.

In Fig. 4, all of the measurements or computed dependencies are shown for an actual or equivalent ball indentation test. The hardness stress is the applied force divided by the contact area, and the hardness strain is the surface projected contact diameter between the ball and the crystal, divided by the ball diameter. A theoretical linear dependence of the elastic Hertzian hardness stress on the indentation strain was computed for the variously positioned "dashed lines" for the different crystals, depending on their elastic constants and those for an assumed steel ball indenter. The solid curve for NaCl was determined experimentally in a continuous indentation test where both the applied load and ball indentation depth were measured. An initial yield point behavior was detected at the onset of plasticity in the NaCl test after which the load was increased until a strain equivalent to a diamond pyramid indentation test result was reached, $(d/D) = 0.375$. Good agreement was found with the separately determined VHN measurement.

The one solid NaCl line in Fig. 4 and other dashed lines are higher as the elastic modulus is greater for each material. Also shown in Fig. 4 as open circle points along the various dashed elastic loading curves are the theoretical (open circle) stresses calculated on an indentation fracture mechanics basis for cracking of the material in the absence of plastic flow [11]. As indicated for the highest MgO result, these stresses are lower for larger ball diameters in agreement with an inverse dependence on the ball diameter. The highest open circle point at the 20 GPa terminus of the MgO elastic loading line is the indentation fracture mechanics stress for cracking with a ball diameter of 0.124 mm, equivalent to the diamond pyramid test values associated with cracking of the material and centered on the lower applied hardness stress of approximately 7 GPa. The stress concentrating action of dislocation pile-ups provides an explanation of the smaller experimental cracking stress [7].

Evaluation of the relative hardness of RDX and the related energetic crystals rests on the comparison of the dashed line positions, for computed elastic loading lines, on the left-hand side of Fig. 4 and the filled circle points on the right-hand side of the figure. For example, the solid elastic loading line for NaCl is above the dashed line for RDX because of the greater NaCl elastic modulus, associated with its ionic bonding, but the greater plastically-determined hardness stresses for RDX, compared to NaCl, occur because of the special intermolecular blockage consideration described in Section 1, earlier. The effect is seen to be greater for PETN than for ionically-bonded AP. Thus, an important aspect of energetic crystal deformation under applied shear stresses is that adjacent atomic outcropping appendages of molecules may be brought into critical reaction coordinate distances under relatively high shear stresses, not far below the value of the theoretical stresses required to cause cracking of the material, as described in Section 1.

2.3. Molecular dynamics analysis of defect-associated hot spots

It is interesting to imagine extension of the preceding, essentially static, deformation considerations to the dynamic deformation and cracking behaviors to be expected for energetic crystals under shock loading conditions. First, there is the consideration of an increase in loading rate on raising the plastic shear strength of energetic crystals, as typical of thermally activated flow for other crystal structure types. However, the small region of stress elevation between the hardness plastic flow stress and the cracking stress for RDX in Fig. 4 leaves little room for further stress elevation, say as compared to the appreciable stress range available for increasing the rate dependent plastic flow strength of NaCl crystals.

Secondly, there is the consideration of the narrow dimensional scale for existence of the shear stress at the shock front in a shock wave experiment. The consideration lends itself to application of the method of molecular dynamics (MD) that, until the recent availability of large machine computations, has been limited by the number of atoms or molecules that could be tracked within a modeled material volume. Nevertheless, the method lends itself at any scale to fundamental calculations of energy partitioning under dynamic loading conditions, and especially provides an opportunity of evaluating defect influences on hot spot development at nanoscale dimensions [12].

Tsai first investigated the role of structural relaxation around defects in generating hot spots in a MD model of a 2D bcc monatomic lattice subjected to 1D shock compression [13]. The model was later extended to a 3D fcc lattice made up of box-like molecules each consisting of eight atoms [14,15]. These model studies indicate that the basic mechanisms for hot spot heating are as follows: (1) defects are local sites of high strain energy, and they reduce the mechanical strength of the lattice; (2) under rapid compression, when the load exceeds the stability of the lattice, structural relaxation would likely begin at some defect site. This relaxation process would convert a part of the strain energy around the defect into kinetic energy of the relaxing atoms and molecules, and thus to local heating; (3) as the relaxing atoms and molecules readjust their positions, they create behind them new defects that would generally require further relaxation. In this way, the relaxing region propagates, usually along easy slip planes, to other parts of the lattice; (4) finally, in a realistic 3D model that could support a number of different modes of defect propagation, the propagating defects could become extensive, and thus, the hot spot could become much larger than the hot spot at the original defect site.

In addition to these mechanisms, the sharing of energies among the translational–rotational–vibrational (T–R–V) degrees of freedom in a molecular crystal was also studied [15]. This problem is important for determining not only the energy equilibration at hot spots, but also the sharing of energies in the T degrees of freedom, from mechanical compression, with the R and V degrees of freedom, i.e. the mechanism of heating in the first place. The MD results would then allow a comparison with those of reference [16] in which the heating process was postulated to be by a mechanism of multi-phonon "up-pumping" through the "doorway" mode from a quantum mechanical viewpoint. It was also postulated in [16] that defects would enhance the anharmonic coupling between T–V and T–R, leading to greater heat transfer to the defect regions, which would then become hot spots.

Reference [15] gives an example of hot spot heating by the mechanisms discussed earlier from the viewpoint of MD. The model consisted of 4088 atoms grouped into 511 molecules and one vacancy. Different Morse potentials were used for the intra and intermolecular interactions, and the intramolecular potential was not too stiff compared with the intermolecular potential. The system was prepared in thermal equilibrium at zero pressure before compression, at time $t = 0$. It was then compressed in the [1 0 0] direction over the entire volume, at a uniform rate, and in one unit of time, such that at the end, the volume was reduced by 10%. In this time, a sound wave would have traveled about the distance of the vacancy. The main results may be summarized as follows. (1) The compression process did not disturb the equilibrium distribution of the energies in the T–R–V degrees of freedom. At the end of compression, $t = 1$, the kinetic temperature of the system increased to 1.34 times the initial temperature (at $t = 0$). (2) Relaxation occurred almost immediately at the end of the compression process, as one of the compressed molecules next to the vacancy defect popped abruptly into the vacant space. This process directly energized the V degrees of freedom of the molecule, although T also increased somewhat. The peak kinetic temperature of this molecule was 3.23 times the initial temperature. From $t = 1$ to $t = 5$, the average kinetic temperature of this molecule remained at about 1.8 times the initial temperature, while the average kinetic temperature of the system remained at 1.34, at least up to $t = 3$. (3) Substantial structural relaxation in the system began around $t = 3$, accompanied by a decrease in the potential energy and a corresponding increase in the kinetic temperature of the system. As the relaxation continued, shear bands were generated. The potential energy released went mostly into the T degrees of freedom. Equipartition of T–R–V was achieved around $t = 15$, which was also the end of structural relaxation. In this case, the heating of the system as a whole from structural relaxation was not large: the average kinetic temperature of the relaxed system at $t = 10$–15 was only 1.48 times the initial temperature, compared with 1.34 before structural relaxation. Still, if there were no structural relaxation after $t = 3$, heating of the system by the single relaxing molecule of (2) would have been much smaller. The results in [14] were similar, except that "kink" lines, from local "buckling", instead of shear bands, propagated throughout the system during structural relaxation, and the heating of the system was much more intense (3.84 times the initial temperature).

These mechanisms for hot spot heating are not in full accord with those discussed in [16]. Enhanced heat transfer undoubtedly occurs at defect sites. But in the MD model here, with a simple vacancy, the hot spot occurred under rapid compression not by enhanced heat transfer, but by the relaxation of some molecule next to the defect; and this heating was augmented by structural relaxation in the crystal on a more global scale. Furthermore, the heating was rapid at the defect site, through the expansion of a compressed molecule into the defect region, directly energizing the V degrees of freedom. These results, however, are incomplete. Additional 3D modeling of hot spots with different interaction potentials, and different types of defects, such as vacancy clusters, dislocations, impurities, grain boundaries, etc. and their movements under different loading, remain to be investigated.

2.4. Hot spots at dislocation pile-up avalanches

All indications are that hot spot sizes of near micrometer dimensions are required for initiation of conventional explosive materials and, as for understanding the deformation properties of structural materials, multiple dislocation movements are necessarily involved in production of hot spots of sufficient size for material initiation. Such consideration led to the dislocation avalanche model of achieving high temperatures associated with the sudden release of a blocked dislocation pile-up [17], as indicated in Fig. 2. Larger hot spot sizes are achieved for such concerted dislocation group interactions.

The dislocation pile-up avalanche model relates also to the prediction of dislocation pile-up-initiated shear banding in structural materials [18]. Fig. 5 shows, in part, a proposed graphical basis that was developed for comparing the shear band susceptibilities of a number of structural materials as related to the top inequality listed in the figure. The symbols used are as follows: *k* for the upper limiting pile-up stress intensity to cause cleavage, *K* is the thermal conductivity, *G* the shear modulus, ***b*** the dislocation Burgers vector, α a number dependent on Poisson's ratio, *l* the crystal or grain diameter, *v* the upper limiting dislocation velocity taken equal to the shear wave speed, and *c* the specific heat at constant volume. The major material parameters in this case are *k* and *K*, hence their ratio, that is designated by the slopes to the open circle points in Fig. 5 give an indication of the material shear band susceptibility. The closed circle points apply for the product of the temperature rise and *K*. On either basis, the model results are seen to be in agreement with the known greater shear banding susceptibilities of aluminum, iron and titanium, in that order.

Also added to Fig. 5 are *k* and *K* points for RDX and several related energetic materials, in their case, based on the combination of material parameters that give the second inequality for the upper limiting dislocation pile-up avalanche behavior. Note that the

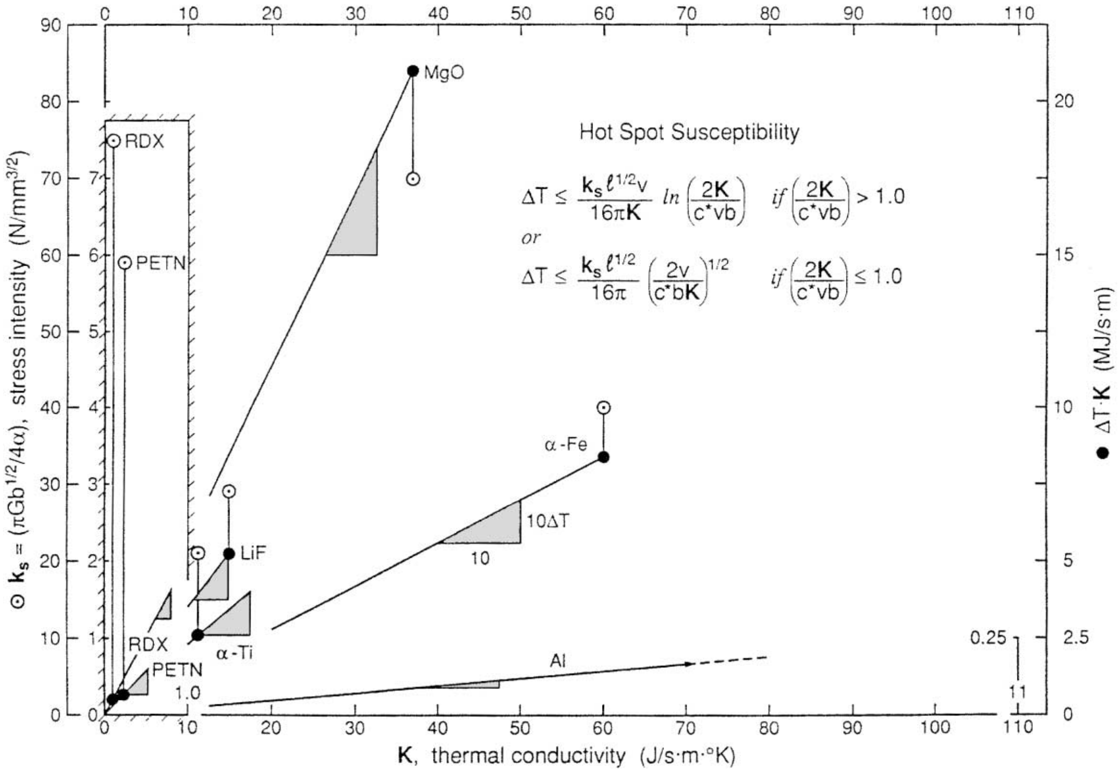


Fig. 5. Theoretical pile-up stress intensity, *k*, vs. thermal conductivity, *K*, for assessing hot spot susceptibility.

Table 1
Hot spot susceptibility estimations for inert and energetic materials[a]

Material	c^* (MJ/m^3 K)	v (km/s)	δx (nm)	G (GPa)	α $(2(1-\nu)/(2-\nu))$	k_s (MPa mm$^{1/2}$)	K (J/s m K)	ΔT (MK)	t_c (ps)
MgO	3.5	6.4	0.30	150	0.91	70	37	0.58	0.85
RDX	2.7	2.1	1.3	7.5	0.88	7.7	0.11	0.51	42
LiF	3.6	5.2	0.28	63	0.90	29	15	0.35	1.9
AP	2.2	1.95	0.75	7.4	0.90	6.3	0.40	0.30	3.1
PETN	1.9	1.75	1.5	5.4	0.88	5.9	0.23	0.27	19
α-Ti	3.0	3.1	0.35	36	0.80	21	11	0.23	3.3
α-Fe	4.5	3.2	0.25	86	0.84	40	60	0.14	0.47
Al	2.7	3.1	0.29	27	0.79	14	210	0.02	0.11

[a] Dislocation pile-up avalanche temperature rises, ΔT, and hot spot lifetimes, $t_c = (\delta x)^2 c^*/K$.

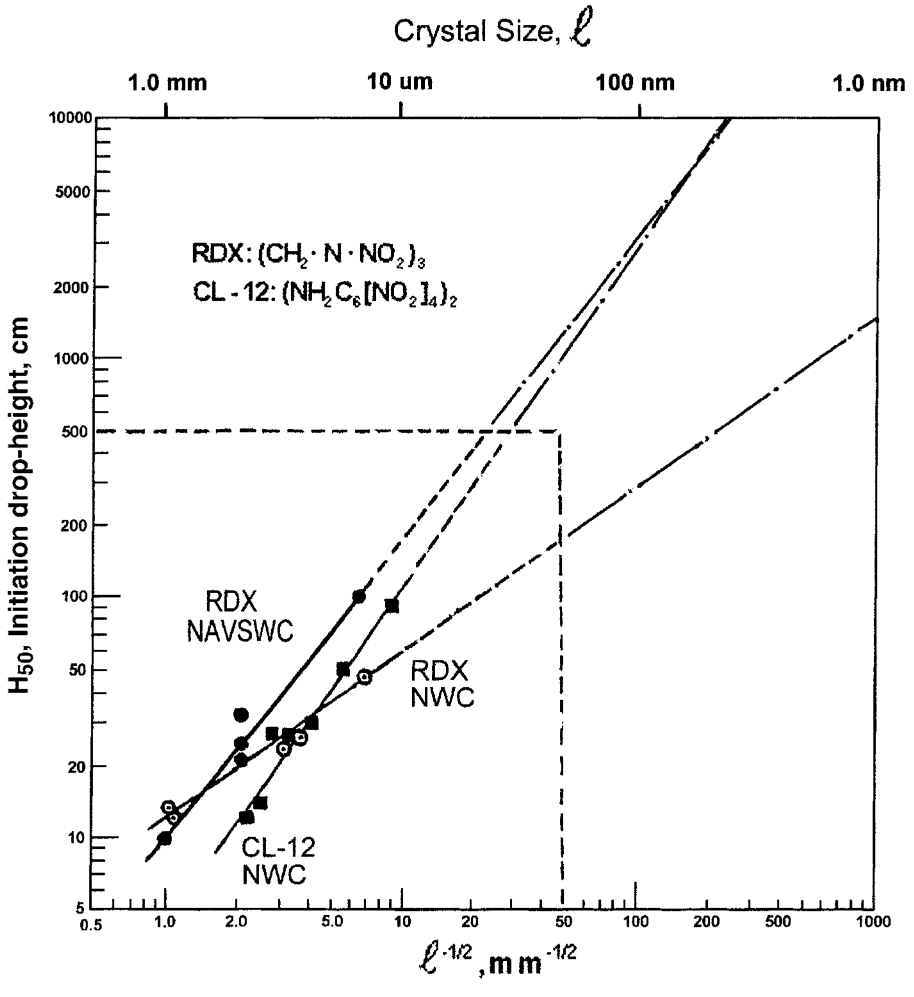


Fig. 6. Crystal size dependence for initiation of RDX and CL-12 in drop-weight impact tests.

respective ordinate and abscissa scales are reduced in direct proportion by an order of magnitude so that comparable graphical behavior can be illustrated. For these materials, and the corresponding pile-up avalanche description, the (*k*/*K*) ratio is not as good an indicator of the effective temperature rise caused by pile-up collapse, as shown by the positions of the filled circle points. However, the comparison of both types of material slopes shows an expected high shear banding susceptibility, and associated hot spot character for RDX and related energetic materials. Such model calculations were carried forward to give the upper limiting temperature rises and hot spot lifetimes shown for the various materials in Table 1. The relative numerical values appear to support the dislocation pile-up avalanche model for generating hot spots in energetic materials.

An important characteristic of the pile-up model is that the strain is non-uniform in the embryonic slip length in accordance with the dislocations being squeezed together more closely at the pile-up tip. When the blocking point is suddenly removed, say by local brittle cracking of a material, the pile-up is released with a magnified driving force on the dislocations closer to the pile-up tip. In this way, the pile-up avalanche model fits the experimental observation of initiation behavior being associated with sudden load reduction in drop-weight impact tests [19]. The temperature rise associated with the modeled pile-up collapse was estimated to be directly proportional to the square root of the crystal slip length, and for the slip length then taken proportional to the crystal size, an inverse square root of crystal size dependence was obtained for the drop-weight height for 50% probability of initiation [20]. Fig. 6 shows reasonable agreement with results obtained for RDX crystals tested at two laboratories and also with various crystal sizes of CL-12 material. Interesting comparison was made also with thermal explosion temperatures, both for PETN and RDX crystals. PETN was determined to be generally more sensitive than RDX because of the lesser thermal stability of the PETN molecule.

The inset dashed square of Fig. 6 was the original publication figure size that has now been extended to consideration of obtaining possibly greater drop-weight height measurements at sub-micrometer crystal dimensions relating to current interest in the study of nanoenergetic materials [21]. Although the lines are easily extended to nanoscale crystal sizes, there are important issues to be resolved of larger dislocation strain energies but lower surface energies occurring for energetic crystals [7], both weighing against obtainment of the extrapolated results. The subject is being further investigated, both experimentally and theoretically.

3. Conclusions

An investigation stimulated by R.S. Miller into the hot spot characteristics of energetic crystals, particularly of RDX and related materials, and on a model basis relating reasonably closely to experimental results, has been a grand experience. The discoveries made, or confirmed, along the investigative way have led to the following conclusions: (1) RDX is relatively hard and brittle for reason of intermolecular blockages to shear deformations that are explained at the crystal lattice level, and that are not alleviated by dislocation movements; (2) nevertheless, molecular dynamics modeling of lattice deformations shows that molecular relaxations associated with dislocation or other defect lattice sites provide significant local hot spot heating; and (3) dislocation pile-up avalanches provide a mechanism for further enhancing hot spot development in tune with known characteristics of RDX and related energetic material sensitivities.

References

[1] R.S. Miller, Research on new energetic materials, in: T.B. Brill, T.P. Russell, W.C. Tao, R.B. Wardle (Eds.), Proceedings of the Materials Research Society Symposium on Decomposition, Combustion and Detonation Chemistry of Energetic Materials, Vol. 418, Pittsburgh, PA, 1996, p. 3.

[2] D.H. Liebenberg, R.W. Armstrong, J.J. Gilman (Eds.), Structure and Properties of Energetic Materials, in: Proceedings of the Materials Research Society Symposium, Vol. 296, Pittsburgh, PA, 1993, p. 3.

[3] R.S. Miller, in: Proceedings of the ONR Workshop on Energetic Material Initiation Fundamentals, Vol. 475, 14–17 October 1986, Los Alamos National Laboratory, NM, Chemical Propulsion Information Agency Publication, 1987.

[4] R.W. Armstrong, in: Proceedings of the ONR/SNPE/ONERA Workshop on Explosive and Propellant Combustion

Mechanisms, 3–4 June 1991, ONREUR Report 91-02-W, July 1991.

[5] A.C. van der Steen, in: Proceedings of the ONR/TNO Prins Maurits Laboratory Workshop on Desensitization of Explosives and Propellants, Vols. 1–3, 11–13 November 1991, TNO preprint.

[6] W.L. Elban, R.W. Armstrong, Microhardness study of RDX to assess localized deformation and its role in hot spot formation, in: Proceedings of the Seventh (International) Symposium on Detonation, NSWC MP 82-334, 1982, p. 976.

[7] R.W. Armstrong, W.L. Elban, Cracking at hardness microindentations in RDX explosive and MgO single crystals, Mater. Sci. Eng. A111 (1989) 35.

[8] J.C. Hoffsommer, D.J. Glover, W.L. Elban, Quantitative evidence for nitroso compound formation in drop-weight impacted RDX crystals, J. Energetic Mater. 3 (1985) 145.

[9] R. Behrens Jr., S. Bulusu, Thermal decomposition of energetic materials. 3. Temporal behaviors of the rates of formation of the gaseous products from condensed phase decomposition of RDX, J. Phys. Chem. 96 (1992) 8877.

[10] R.W. Armstrong, H.L. Ammon, Z.Y. Du, W.L. Elban, X.J. Zhang, Energetic crystal-lattice-dependent responses, in: Proceedings of the Materials Research Society Symposium, Vol. 296, Pittsburgh, PA, 1993, p. 227.

[11] B.L. Hammond, R.W. Armstrong, Recovered elastic and plastic strains at residual microindentations in an MgO crystal, Philos. Mag. Lett. 57 (1988) 41.

[12] D.H. Tsai, Hot spot heating from impurities and vacancies in a crystalline solid under rapid compression, in: Proceedings of the Materials Research Society Symposium, Vol. 296, Pittsburgh, PA, 1993, p. 113.

[13] D.H. Tsai, Structural defects and 'hot spot' formation in a crystalline solid under rapid compression. I. Vacancy clusters and slip bands, J. Chem. Phys. 95 (1991) 7497.

[14] D.H. Tsai, R.W. Armstrong, Defect-enhanced structural relaxation mechanism for the evolution of hot spots in rapidly compressed crystals, J. Phys. Chem. 98 (1994) 10997.

[15] D.H. Tsai, Hot spots in a molecular solid under rapid compression: energy sharing among the T–R–V degrees of freedom, in: Proceedings of the Materials Research Society Symposium on Decomposition, Combustion and Detonation Chemistry of Energetic Materials, Vol. 418, Pittsburgh, PA, 1996, p. 281.

[16] A. Tokmakoff, M.D. Fayer, D.D. Dlott, Chemical reaction initiation and hot-spot formation in shocked energetic molecular materials, J. Phys. Chem. 97 (1993) 1901.

[17] R.W. Armstrong, C.S. Coffey, W.L. Elban, Adiabatic heating at a dislocation pile-up avalanche, Acta Metall. 30 (1982) 2111.

[18] R.W. Armstrong, F.J. Zerilli, Dislocation mechanics aspects of plastic instability and shear banding, Mech. Mater. 17 (1994) 319.

[19] S.N. Heavens, J.E. Field, The ignition of a thin layer of explosive by impact, Proc. R. Soc. London A338 (1974) 77.

[20] R.W. Armstrong, C.S. Coffey, V.F. DeVost, W.L. Elban, Crystal size dependence for impact initiation of RDX explosive, J. Appl. Phys. 68 (1990) 979.

[21] W.H. Wilson, M.P. Kramer, R.W. Armstrong, Air Force research in nanoenergetics—potential advantages and challenges, in: Proceedings of the 221st ACS National Meeting, San Diego, 1–5 April 2001.