Initiation of Energetic Materials: From Intermolecular Shearing to Nano-Composite Behavioral Predictions

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Extended Abstract

The essentially static indentation hardness properties of energetic and related inert crystals, including those load – displacement dependences measured in nanoindentation tests, are assessed in relation to modeling of the crystal elastic/plastic/cracking behaviors; and, these results, in turn, are related to the broad dynamics of crystal size-dependent material initiation properties that are measured in drop-weight impact tests or in associated compaction or combustion tests or, at highest deformation rates, in shocks or shock-less isentropic compression tests. The description of modeled material initiation behaviors encompasses considerations of: (1) dislocation-assisted intermolecular reactions within the crystal lattice; (2) hot spot generation via crystal size dependent dislocation pile-up avalanches; (3) incorporation of Arrhenius-type dislocation-based constitutive deformation behaviors; and, (4) a role for dislocation-generated plasticity and cracking in determining porosity-dependent composite material compaction and resultant test measurements.

Prior indentation fracture mechanics measurements made of surface energy evaluations for cracking at diamond pyramid indentations put into RDX (cyclotrimethylenetrinitramine) crystal surfaces[1] gave evidence that, when compared to corresponding thermodynamic values of surface energy[2], cleavage cracking was occurring at relatively low applied stresses. Follow-up observations of restricted dislocation etch pit zones surrounding hardness impressions put into RDX crystal surfaces, as compared with LiF indentations, provided evidence of special difficulty in dislocation movement in the former lattice structure[3]. Thus, these results, taken together with the relatively weaker molecular bonding between individual covalently-bonded molecules in the RDX crystal lattice led to the description of it and related (high explosive) energetic crystals being elastically compliant, plastically strong, and prone to cleavage cracking[4]. The combined measurements of elastic/plastic/cracking behaviors are graphically demonstrated through development of hardness-determined stress-strain curves[5]. An important consequence for energetic crystals is that there is a relatively narrow range in stress for dynamic material behavior between the material static yielding and subsequent cracking behaviors.

Model descriptions are presented of elementary shearing displacements that bring outcropping appendages of adjacent RDX molecules into critical reaction coordinate distances and, also, of differentiation between preferred deformation mechanisms of easier slip on ~(040) planes as compared with more difficult slip on (021) planes. In the latter case, the modeled intermolecular interactions are associated with nitroso compound formations detected in post-analysis of "no go" drop-weight tested RDX particle materials[6]. The RDX slip results are compared with an alternative deformation twinning response in the (cyclotetramethylenetetranitramine) HMX crystal lattice[7]. An update is given of the key feature of plasticity-assisted hot spot development in RDX and related energetic and (shear band prone) inert crystal structures based on the breakthrough of dislocation pile-up avalanches when overcoming barrier-type obstacles sufficiently strong to result in cleavage cracking[8]; and, which model consideration leads to prediction of an inverse square root of crystal size dependence for drop-weight impact height measurements of energetic crystal sensitivities[9].

The crystal size dependent drop-weight sensitivity measurements relate also to modeling of an analogous particle size effect in the combustion behaviors of compacted HMX particle beds[10]. In general, a benefit of greater insensitivity to initiation is predicted for finer crystal/particle size materials, even when reduced to nanometric dimensions, and, once initiated, an advantage of greater power dissipation is also achieved. The occurrence of relatively more complicated strength behaviors being predicted either for dislocation generations in shock tests or drag-controlled dislocation velocities in equally high rate but shock-less isentropic compression tests of energetic or related inert materials are assessed in terms of constitutive equation descriptions involving a role for a dislocation-forcing-type shear stress in the Gibbs free energy term of an Arrhenius-type equation, not unrelated to those equations employed for thermal descriptions of hot spot developments[11]. Even the influence of porosity in formulated energetic composite materials is reasoned to have plasticity-associated dislocation consequences at lower stress than required for the onset of instability by surface jetting. And, lastly, there is the proposed importance of the material contiguity parameter in evaluating the strengthening and/or cracking pressures associated with mutually impinging hard (RDX) particles within the highly-filled and softer (polymer) matrices of energetic composite material formulations[12].

References

1. J.T. Hagen and M.M. Chaudhri, "Fracture surface energies of high explosives", J. Mater. Sci. 12, pp. 1055-1058, 1977.

2. W.L. Elban, "Surface energies of high explosives PETN and RDX from contact angle measurements", J. Mater. Sci. (Lett.) 14, 1008-1011, 1979.

3. W.L. Elban and R.W. Armstrong, "Microhardness study of RDX to assess localized deformation and its role in hot spot formation", Seventh Symp. (Intern.) on Detonation, NSWC MP 82-334, pp. 976-985, 1982.

4. R.W. Armstrong and W.L. Elban, “Dislocations in energetic crystals”, in Dislocations in Solids, Eds: F.R.N. Nabarro and J.P. Hirth, 12, pp. 403-446, Elsevier Sci. Publ. B.V., Oxford, 2004.

5. R.W. Armstrong and W.L. Elban, “Macro- to nano-indentation hardness stress-strain aspects of crystal elastic/plastic/cracking behaviors”, Exp. Mech. DOI: 10.1007/s11340-009-9246-5, 2009.

6. J.C. Hoffsommer, D.J. Glover and W.L. Elban, “Quantitative evidence for nitroso compound formation in drop-weight impacted RDX crystals: J. Energ. Mater. 3, pp. 149-158, 1985.

7. R.W. Armstrong, H.L. Ammon, Z.Y. Du, W.L. Elban and X.J. Zhang, “Energetic crystal-lattice-dependent responses”, in Structure and Properties of Energetic Materials, Eds: D.H. Liebenberg, R.W. Armstrong, and J.J. Gilman, 296, pp. 227-232, Mater. Res. Soc., Pittsburgh, PA, 1993.

8. R.W. Armstrong, C.S. Coffey and W.L. Elban, “Adiabatic heating at a dislocation pile-up avalanche”, Acta Metall. 30, pp. 2111-2116, 1982.

9. R.W. Armstrong, C.S. Coffey, V.F. DeVost and W.L. Elban, “Crystal size dependence for impact initiation of RDX explosive”, J. Appl. Phys. 68, pp. 979-984, 1990.

10. R.W. Armstrong and W.L. Elban, “Materials science and technology aspects of energetic (explosive) materials”, Mater. Sci. Tech. 22, pp. 381-395, 2006.

11. R.W. Armstrong, W. Arnold and F.J. Zerilli, “Dislocation mechanics of copper and iron in high rate deformation tests”, J. Appl. Phys. 105, 023511, 2009.

12. R.W. Armstrong, “Dislocation mechanics aspects of energetic material composites”, Rev. Adv. Mater. Sci. 19, pp. 13-40, 2009.