PHYSICAL REVIEW B VOLUME 60, NUMBER 13 1 OCTOBER 1999-I

Plastic deformation, energy dissipation, and initiation of crystalline explosives

C. S. Coffey
Indian Head Division, Naval Surface Warfare Center, Indian Head, Maryland 20640-5035

J. Sharma
Carderock Division, Naval Surface Warfare Center, Carderock, Maryland 20817

(Received 22 October 1998)

This is an effort to understand plastic deformation and energy dissipation in crystalline solids during shock or impact. It builds on recent atomic force microscope observations that plastic flow creates localized distortions in the lattice and molecules of at least some classes of molecular crystals. A distorted lattice potential is developed through which the dislocations responsible for plastic flow move by quantum tunneling. Plastic strain and energy dissipation rates are determined and related to crystal size and damage. These account for plastic flow in crystalline solids and the initiation of chemical reactions in crystalline explosives subjected to shock or impact. The predictions are compared with experiments. [S0163-1829(99)13133-3]

INTRODUCTION

This is an effort to understand plastic deformation and energy dissipation in crystalline solids during shock or impact loading. Recent atomic force microscope (AFM) investigations of the lattice and molecular structure of molecular crystals that had undergone plastic deformation due to impact or shock have revealed a variety of complex behaviors including considerable distortion of both the lattice and molecules.[1–3] The AFM investigations were mainly on the molecular crystal RDX ($C_3H_6N_6O_6$). RDX is an explosive material, however chemical reactions were only observed at higher levels of impact or shock. The results are similar to less complete AFM records of the crystalline explosives HMX ($C_4H_8N_8O_8$) and TATB ($C_6H_6N_6O_6$) and are believed to be representative of deformations in nonexplosive crystals as well.

With increased loading the RDX molecules were increasingly deformed, shifted, and rotated out of their equilibrium positions. The nature of this disorder appears to remain the same regardless of the amplitude of the applied load. The distorted lattice and molecules were found in localized regions of high plastic deformation often referred to as shear bands. When chemical reactions occurred they were observed to originate in the heavily deformed shear band regions.

It is appreciated that the AFM examines only the crystal surfaces and that the current data is preliminary. However, in this work a large number of surfaces were examined, including many known to have been in the interior of the crystals during plastic flow. Without exception, all surfaces revealed similar images suggesting that similar patterns persist throughout the damaged crystals.

DISORDERED LATTICE AND MOLECULES

Here it will be assumed that both the lattice and molecular distortions due to shock or impact induced deformation are concentrated in localized shear bands throughout the interior of the crystal. The distortion of the lattice and the molecules is attributed to the presence of the dislocations responsible for plastic flow. With the creation of each dislocation, the molecules lying on the slip plane of the newly created dislocation are displaced by the presence of the dislocation core. Since to first order the size of the crystal remains nearly constant during shear deformation, these molecules are compressed by this displacement and must attain new lowest energy states and spatial configurations. With the creation of increased numbers of dislocations on an active slip plane the molecules and lattice on the slip plane experience increased amounts of distortion. Since the sources that create dislocations are likely to intersect a number of adjacent slip planes it is hypothesized that these adjoining slip planes combine to form narrow shear band regions of often intense plastic deformation.

Let U be the potential energy of the distorted lattice. When N dislocations, created during plastic flow, are inserted onto the active slip plane the average potential of the distorted lattice along the slip plane can be approximated as

$$U = U_0 + \frac{dU_0}{dN} N + \cdots, \tag{1}$$

where U_0 is the undistorted portion of the lattice potential. The distorted part of the potential can be rewritten as $dU_0/dN = (dU_0/dx)(dx/dN)$. For an undistorted lattice, $dU_0/dx = 0$.[4] However, for a disordered lattice, $dU_0/dx \neq 0$, but is a measure of the average amount of damage imparted to the crystal by the deformation. Implicit here is that $N = N(t)$ and the time required to create and move these dislocations on the slip active planes must be taken into account. This has important implications for the response of crystals to fast shocks.

If the core of each dislocation introduces a displacement δ onto the active slip plane and if on average each molecule or atom on the active slip plane in their new equilibrium position is compressed equally, then on an active slip plane

$$\frac{dx}{dN} = \frac{\delta d}{\ell}, \tag{2}$$

where ℓ is the length of the crystal and d is the molecular spacing of the undeformed lattice so that ℓ/d is the number of molecules/atoms on the slip plane. The distorted lattice potential can now be written as

$$U=U_0+\frac{dU_0}{dx}\frac{\delta d}{\ell}N. \tag{3}$$

This is the average potential of the deformed lattice in terms of the undeformed lattice potential, number of dislocations, crystal particle size, and the average damage term dU_0/dx.

QUANTUM MECHANICAL APPROACH TO PLASTIC FLOW IN DISORDERED CRYSTALS

In their classic paper Kocks, Argon, and Ashby determined the constitutive relations describing slip in crystalline solids.[5] Fundamental to this description is the process of thermal activation by which a dislocation moving with energy E in the crystal can overcome a barrier of energy U when $U>E$. In classical physics when such obstacles are encountered dislocation motion and plastic flow are halted. These obstacles can be overcome when the energy of the dislocation combined with that of the thermal fluctuations exceeds the energy of obstacle, so that temporarily $E+E_{\mathrm{th}}>U$. However, this classical approach limits the description of plastic deformation to relatively low rate processes because at room temperatures the thermal fluctuations occur at frequencies $\leqslant 10^{11}\,\mathrm{s}^{-1}$.[5,6] But during strong shock or impact the dislocations move at velocities approaching the local shear wave speed and encounter and pass the lattice barriers at rates of $10^{13}\,\mathrm{s}^{-1}$.[7,8] Thus it is unlikely that thermal fluctuations can have a major role in plastic deformation at high rates due to strong shock or impact.

The movement of a dislocation occurs by shifting and rearranging the electron bonds that establish the lattice near the dislocation core. This is necessarily a quantum-mechanical process. Often, however, dislocation motion can be approximated by classical Newtonian mechanics in the limit of a large dislocation effective mass and a broad, well characterized, potential barrier.[9] Here, a quantum-mechanical description is developed which approximates the asymptotic behavior of dislocation motion over the range from very low to very large shear stress including the transition region between these asymptotic regions.

Rather than wait until a thermal fluctuation gives them the energy necessary to surmount the lattice potential barriers, the dislocations move by quantum tunneling through the potential barriers.[10,11] Tunneling enables the dislocations to transit the lattice potential barriers at rates in excess of $10^{13}\,\mathrm{s}^{-1}$ necessary for plastic flow to occur due to strong shock or impact. Unlike the classical picture, in the quantum picture the lattice potential determines dislocation motion even when $E>U$.

DISLOCATION VELOCITY

In the tunneling picture the dislocation core is treated as a pseudoparticle.[10,11] The velocity of the dislocation through the lattice is determined in part by the probability T that the dislocation core will tunnel through the potential barrier of the surrounding lattice and transit into the adjacent lattice site. The dislocation velocity is $v=v_0T$ where v_0 is the local shear wave speed.[10,11] At high shear stress levels, where $T\rightarrow 1$, the maximum dislocation velocity approaches the local shear wave speed $v\rightarrow v_0$. This is in agreement with the observations that the velocity of the plastic wave due to high amplitude shocks approaches v_0 and is expected since the plastic wave is formed by the moving dislocations.[7]

EFFECT OF PARTICLE SIZE ON WIDTH OF POTENTIAL BARRIER

In addition to affecting the height of the lattice potential barrier the presence of dislocations also reduces the thickness of the potential barrier where substantial tunneling occurs. This can happen because the increased barrier height will cause tunneling to occur at greater dislocation energy where the barrier will be thinner. Also, compression of the lattice and molecules by the dislocations acts to decrease the size of the molecules and reduces the thickness of the lattice potential barrier.

To illustrate the effect that reducing the thickness of the potential barrier has on the tunneling probability, consider an idealized rectangular lattice potential. Let W be the barrier thickness and W_0 be the barrier thickness when the particle size is very large and has no role in increasing the height of the barrier. Assume a simple approximate form for the width of the barrier

$$W=W_0\left(1-\frac{\beta N\,\delta d}{W_0\ell}\right), \tag{4}$$

where β is a constant and $W\geqslant 0$.

DISLOCATION TUNNELING

Only the conditions for substantial plastic flow and energy dissipation will be of concern here. Typically, the effective mass of a dislocation is large, much greater than the electron mass, so that only the region near the top of the potential barrier is of interest. For simplicity, the average potential barrier will be represented by a rectangular barrier. When the energy of the moving dislocation E is less than the height of the potential barrier $E<U$ the probability of tunneling is[12]

$$T=\frac{4E(U-E)}{4E(U-E)+U^2\sinh^2\zeta(U-E)^{1/2}W}, \tag{5}$$

where $\zeta=(2m/\hbar^2)^{1/2}$, $\hbar$ is Planck's constant, m is the effective mass of the dislocation, and

$$E=\tfrac{1}{2}\frac{\tau^2}{G}V+\tfrac{1}{2}k\Theta, \tag{6}$$

where τ is the applied shear stress, G is the shear modulus, Θ is the temperature, k is Boltzmann's constant, and V is the volume of the dislocation core. When $E>U$ the motion of the dislocations is determined by a modification of Eq. (5).[12]

Summarizing, Eqs. (3), (4), (5), and (6) predict that an increased shear stress is required to achieve tunneling and plastic flow with decreased particle size. However, the τ^2 dependence of the dislocation energy and the diminished potential barrier thickness with decreased crystal size result in a more rapid transition toward $T \rightarrow 1$ with this increased shear stress. These behaviors are not found in the classical analyses.

PLASTIC DEFORMATION RATE

In an earlier work, a simple generic source was proposed to create dislocations in which the rate of creation was principally determined by the inverse of the time required for a dislocation moving at a velocity v to transit a source of size ℓ_s:[13]

$$\frac{dN}{dt} = 2\frac{V}{\ell_s} p_c . \tag{7}$$

p_c is the probability of creating a dislocation and the factor 2 takes into account the creation of a pair of dislocations. Integrating Eq. (7) with respect to time and combining with the Orowan expression for the plastic strain rate gives the plastic strain rate in terms of the tunneling probability that the dislocations will transit the lattice potential barrier and move through the lattice as[10,11,14]

$$\frac{d\gamma_p}{dt} \approx \frac{2T(\tau) v_0 b p_c N_s \ell}{\ell_s} . \tag{8}$$

N_s is the number of dislocation sources that have created the dislocations responsible for the plastic strain.

ENERGY DISSIPATION BY MOVING DISLOCATIONS

Energy dissipation occurs simultaneously with plastic flow. The dislocations perturb the lattice as they move giving rise to energy dissipation and local heating within the lattice. Keeping just the lead terms, the local energy dissipation rate can be approximated as[15,16]

$$\frac{dE}{dt} \approx A v_0 T(\tau) + \prod_{\ell=0} \frac{B_\ell}{\left[E_\ell - E_{\ell-1} - T(\tau)\dfrac{\hbar v_0}{d}\right]^2 + \Gamma_\ell^2}, \tag{9}$$

where A and B_ℓ are constants given in Refs. (15) and (16). Γ_ℓ is the width of the ℓth internal molecular vibrational level.

The first term in Eq. (9) accounts for energy dissipation due to slower moving dislocations typical of mild shock or impact when $T(\tau) < 1$. It resembles the classical expression for the energy dissipation by moving dislocations,[5] but with emphasis on the more fundamental tunneling probability.

The second term above accounts for the possible resonant excitation of the molecular internal vibrational modes by rapidly moving dislocations. The resonant denominator contains the quantity $E_\ell - E_{\ell-1}$ which is the energy difference between the ℓ and $\ell - 1$ internal molecular vibrational modes. For typical molecular solids $(E_\ell - E_{\ell-1})/\hbar \approx 10^{13}$ rad/s. A moving dislocation encounters and perturbs the lattice v/d times per second. These perturbations generate phonons in a band centered at a frequency of $\omega_0 = 2\pi v_0 T(\tau)/d$. For a typical crystalline explosive $v_0 \approx 2 \times 10^3$ m/s and $d \approx 5 \times 10^{-10}$ m so that $\omega_0 \approx 10^{13} T(\tau)$ rad/s. A dislocation moving in a realistic lattice potential will generate even higher energy phonon components in the side band above ω_0. Thus, for a strong shock where $T(\tau) \rightarrow 1$, the rapidly moving dislocations can resonantly excite the internal vibrational modes of the neighboring molecules. It is reasonable to assume that the density of internal molecular vibrational states is sufficient in most complicated disordered molecular crystals so that intermediate and final states are always available and the rapidly moving dislocations can produce resonant multiphonon excitation and even molecular dissociation in times $\leqslant 10^{-10}$ s.[15–18] This fast molecular dissociation as $T(\tau) \rightarrow 1$ is responsible for the rapid release of stored chemical energy characteristic of detonation in energetic materials.

COMPARISON WITH EXPERIMENT

Next, these results will be used to predict plastic flow and energy dissipation in simple ductile metals and in molecular crystals. A rectangular lattice potential barrier will be assumed so that the tunneling probability is given by Eq. (5). To assure a uniform behavior regardless of particle size, it will be assumed that the nature and operation of the dislocation sources and the local energy density required to start chemical reaction are independent of crystal size.

SIMPLE METALS

Briefly, for simple metals the onset of significant plastic flow occurs when $E \rightarrow U$. Combining Eqs. (3) and (6) gives the approximation that $\tau \approx [\tau_Y^2 + \kappa/\ell]^{1/2}$ which reproduces the Hall-Petch empirical result relating the shear stress for plastic flow with particle size.[19,20] A more complete description of plastic deformation is contained in Eq. (3) to (8). Included are the predictions that deformation of small metal particles requires a greater shear stress and is characterized by a more rapid transition to $T(\tau) \approx 1$ and a more rapid increase in energy dissipation than plastic deformation of the same metal in larger particle sizes. The plastic deformation rate, Eq. (8), reproduces the observed response for several metals including the characteristic deformation behavior at both small and large shear stresses which is determined by the asymptotic behavior of the tunneling probability.[10,11,21,22] For metals there are no internal molecular vibrational modes and energy dissipation is only due to the first term in Eq. (9). Often, because of thermal diffusion processes, the effects of heating in metal particles are difficult to follow directly and limited in response time.

CRYSTALLINE EXPLOSIVES

The response of explosive crystals to shock or impact is of special interest because the localized energy dissipated in these molecular crystals as they undergo rapid plastic deformation is likely to cause the initiation of chemical reaction including the very rapid resonant excitation typical of detonation as $T(\tau) \rightarrow 1$. This allows the predicted plastic flow and energy dissipation-initiation response of explosive crystals to be directly compared with the extensive set of experimental observations relating the initiation behavior of explosive crystals to particle size, damage, shock strength, and the rate of loading.

The energy supplied by mild shock or impact is usually insufficient to raise the energy of the bulk of the explosive to

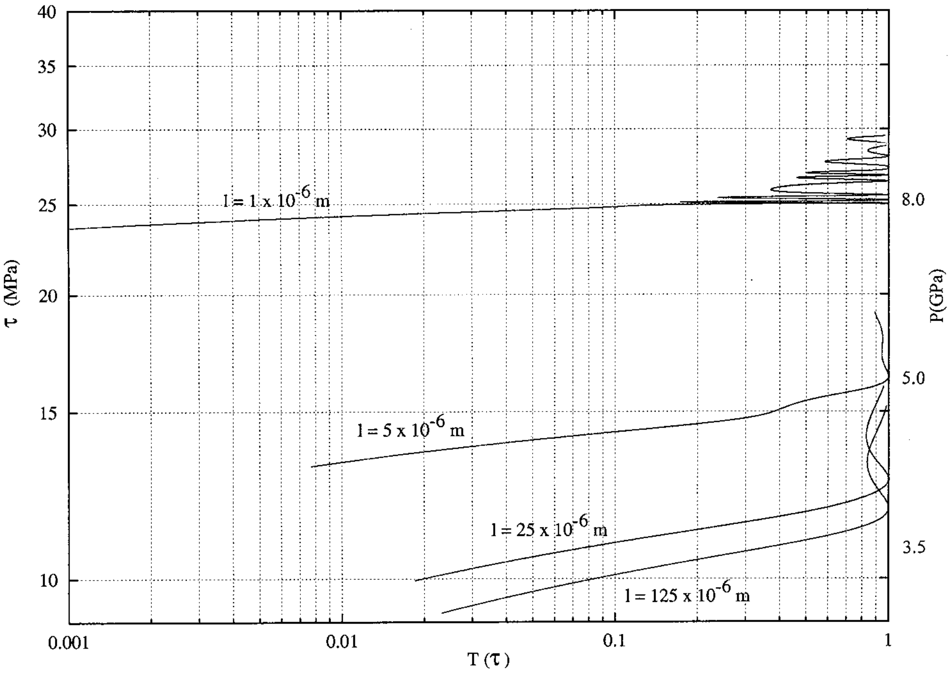

FIG. 1. Shear stress vs tunneling probability for several different size HMX crystals. Calculations are from Eq. (5) and data given in Appendix. The plastic strain rate is $d\gamma_p/dt \approx 5\times10^5 T(\tau)$. Initiation of chemical reaction starts at about $T(\tau)\approx .1$ and detonation threshold occurs when $T(\tau)$ first approaches unity. Pressure levels where $T(\tau)$ first approaches unity are shown on the right-hand side. Detonation occurs for all shear stress levels where $T(\tau)\approx 1$.

levels where reaction can start. In the case of strong shock there is substantial experimental evidence and engineering experience that plastic flow is necessary for initiation of detonation to occur. If plastic flow is suppressed, as occurs when an explosive is pressed to crystal density and inertially confined, reaction does not occur at any reasonable shock pressure, $P < 30-50\,\mathrm{GPa}$.[23–27] The role of pressure in initiation is mainly to generate the required plastic flow and energy dissipation.

Consider first plastic flow and energy dissipation rates in the organic crystalline explosives RDX and HMX. Using typical inputs given in the Appendix, Fig. 1 shows the tunneling probability as a function of the applied shear stress for several different crystal particle sizes for the explosive HMX. From Eqs. (8) and (9) the plastic strain rate is $d\gamma_p/dt \approx 8\times10^5 T(\tau)\,\mathrm{s}^{-1}$ and the energy dissipation rate, $dE/dt \approx N\ [.9\times10^{-11}T(\tau)+\text{resonant terms}]$ J/ms, where typically at high deformation levels $N\approx10^{10}-10^{12}$ dislocations per m^2.[28] Initiation of chemical reaction occurs when the local energy density due to dissipation exceeds the reaction threshold energy density. Maximum plastic flow, dissipation, and reaction rates occur as $T(\tau)\rightarrow 1$.

Figure 1 illustrates the role that particle size can have in increasing height of the lattice potential barrier. A greater shear stress is required to achieve plastic flow via tunneling and to initiate reaction in a small particle size explosive composition than in an identical composition containing larger particles. In practice, small explosive crystals are often used to achieve insensitive explosive compositions. The oscillations that occur as $T(\tau)\rightarrow 1$, shown in Fig. 1, are due to the tunneling process since dislocation motion is still determined by the lattice potential even though $E > U$. Because most explosives are aggregates of randomly orientated explosive crystals these oscillations are expected to average to zero over the bulk of the solid.

While explosive compositions containing small particle size crystals are more difficult to initiate, they transition to detonation more rapidly than larger crystals of the same material. As noted above, this occurs because the dislocation energy increases as τ^2 so that for a small increase in shear stress $T(\tau)\rightarrow 1$ more rapidly at the higher shear stresses required for substantial dislocation tunneling in small crystals than at the lower shear stress levels needed to deform larger size crystals. This is illustrated by the slope $[dT(\tau)/d\tau]^{-1}$ for the different particles sizes as shown in Fig. 1. For this reason, small particle size explosives are sensitive to initiation by high amplitude, short duration, shock pulses. To minimally initiate detonation in large particle size explosive compositions requires a lower amplitude but longer duration shear stress. This effect has been observed in many explosive materials including the 5 μ and 300 μ compositions in Fig. 1. In this way, particle size influences the reaction rate and the curvature of the detonation front in an explosive charge.[29,30]

The detonation threshold shear stress levels for different size HMX crystals are determined from Eq. (5) and the condition where $T(\tau)$ first approaches unity. Experimentally, the shock pressure level for which detonation first occurs is determined by a standard shock test.[31] The shear stress level at which detonation occurs is proportional to the detonation threshold shock pressure.[32] In order to compare the above predictions with experimental results, the measured detonation threshold pressure of the explosive PBXN-110 ($\langle \ell \rangle \approx 300\,\mu$), $P_{\mathrm{th}}\approx 3.5\,\mathrm{GPa}$, has been used to establish a simple scaling relation between the measured shock initiation pressure and the calculated detonation threshold shear stress.[33]

TABLE I. Detonation initiation pressure [HMX, LSGT (Ref. 31)].

Particle size $l(\mu)$	Calc. initiation Shear, τ_l(MPa)	Calc. initiation Pressure, P_l(GPa)	Observed initiation Pressure (GPa)
300.0	10.96	3.5 (PBXN-110)	3.5
5.0	15.85	5.06 (PBXN-128)	4.8
5.0	15.85	5.06 (EXP-3)	4.9
4.0	18.6	5.94 (EXP-4)	6.0
2.5	22.4	7.15	*[a]
1.0[b]	25.1	8.02	*[a]

[a] The detonation threshold pressures for these materials have yet to be measured.

[b] Reference 34.

Here, the scaling constant circumvents the need to establish the reaction threshold level and to properly treat the polymer binder that usually encapsulates the explosive crystals. The same scaling constant was used to determine the detonation threshold shock pressures from the calculated detonation shear stress levels for all of the materials shown in Fig. 1 and in Table I.

In another set of experiments, identical compositions based on the explosive RDX were employed and only the RDX particle size was varied.[30] Both the predicted increase in the shear stress required to initiate reaction and the more rapid transition to detonation were observed with decreasing RDX particle size. The predicted and measured detonation threshold stresses are listed in Table II. In the calculations that resulted in Fig. 1 and Tables I and II, only the particle size has been allowed to change, the remaining inputs are the nominal RDX or HMX properties given in the Appendix. The differences between the predicted and the observed detonation threshold pressures are less than 5% while the particle size varied by two orders of magnitude.

THE ROLE OF SHEAR IN THE INITIATION OF AMMONIUM PERCHLORATE

To further illustrate the role of shear, plastic deformation, and particle size in initiating chemical reaction, consider the energetic material ammonium perchlorate, AP (NH_3ClO_4). In large particle sizes this material cannot be detonated at what are considered reasonable pressures and has been deemed safe to store and transport as an oxidizer. However, in a small particle size, $\leqslant 3\times10^{-5}$ m, AP readily detonates and is recognized as a hazard. The reasons for this behavior are given above. AP has no fuel component to sustain reaction, so that large AP crystals usually heat and disintegrate before high shear stress levels are developed so that $T(\tau)$ never approaches unity and detonation does not occur.[36] In the case of small AP particle size, a higher shear stress amplitude is required for substantial plastic flow to occur. However, once plastic flow begins, only a slight increase in the applied shear stress is required to cause the transition to $T \approx 1$. Now the internal molecular modes of the AP molecules can be resonantly excited resulting in rapid molecular dissociation and release of stored chemical energy in times typical of detonation. This behavior is found in other energetic materials which also lack the fuel or oxidizer components to sustain low level reactions due to impact or moderate shock but can readily be made to detonate at high shock pressure and small particle size.

TABLE II. Detonation initiation pressure [RDX, wedge test (Refs. 30 and 35)].

Particle size, $l(\mu)$	Calc. initiation Shear, τ_l(MPa)	Calc. initiation Pressure, P_l(GPa)	Observed initiation Pressure (GPa)
6.0	15.8	12.0	12.0
135.	11.75	8.9	8.5
428.	10.0	7.6	**[a]

[a] Broad transition centered at about 7–8 GPa.

INITIATION BY IMPACT AND MILD SHOCK

The processes by which explosives are initiated by impact and mild shock have never been understood. Here, this is remedied by treating impact and mild shock as extensions of the above relations into the regime where $T(\tau)<1$.

The plastic deformation rate of HMX crystals subjected to impact or mild shock has been examined over the range $10^{-5}\ \mathrm{s}^{-1} < d\gamma_p/dt \leqslant 10^{5}\ \mathrm{s}^{-1}$.[37] Reaction initiation likely occurs over the range $.01 \leqslant T(\tau) \leqslant 1$. Vigorous reaction during impact and mild shock starts at plastic strain rates somewhat less than $10^5\ \mathrm{s}^{-1}$ [where $T(\tau)\approx .1$] and violent reactions have been noted near $d\gamma_p/dt = 10^5\ \mathrm{s}^{-1}$, [$T(\tau)\approx .2$].[37,38] The predicted strain rate at which detonation occurs is $d\gamma_p/dt \approx 5\times10^5\ \mathrm{s}^{-1}$, [$T(\tau)=1$]. The violent but less than detonation reactions that occur near $d\gamma_p/dt = 10^5\ \mathrm{s}^{-1}$ are due to energy dissipation arising from contributions mainly from the impact term but partially from the resonant term in the energy dissipation rate.

SUMMARY

A complete description of the motion of dislocations in crystalline solids requires a quantum-mechanical analysis. This is particularly the case for the high rates of plastic deformation due to shock or impact. A disordered lattice potential has been derived that incorporates the extent of plastic deformation, particle size, and crystal damage. Plastic flow is determined by the probability that a dislocation core will tunnel through the disordered lattice potential.

Good agreement has been obtained between theory and experiment even with the use of a simple rectangular lattice potential barrier. The response of crystalline explosives to impact and mild shock has been determined and has been related to the response of the explosive crystals to strong shock and detonation. Also, the roles that crystal particle size, damage, temperature, and the extent of plastic deformation have in initiating chemical reaction in crystalline explosives have been determined.

Both the predicted and observed particle size behavior of the reaction initiation threshold of explosive crystals imply that, during shock or impact, dislocations are created and move through the crystals for periods of several transit times ℓ/v before reaction starts. During this time the crystals must retain their integrity. Thus initiation by shock or impact is primarily a solid-state process. It is not until after chemical reaction has reduced the major portion of crystalline explosives to their gaseous components that continuum hydrodynamics can play an important role in determining further explosive response.

ACKNOWLEDGMENTS

C.S.C. wishes to acknowledge the support of the Independent Research Program of the Indian Head Division of NSWC and J. S. wishes to acknowledge the support of the Office of Naval Research. They also want to thank Professor R. W. Armstrong, Professor W. L. Elban, Dr. R. E. Lemar, and G. Sutherland for many discussions on this topic and Dr. K. F. Mueller and S. E. Mitchell for their support.

APPENDIX

In order to compare these predictions with experiments using crystals of different sizes it will be assumed that the sources that create the dislocations are independent of crystal particle size. Also, it will be assumed that the number of sources per unit cross sectional area of crystal is a constant, independent of crystal particle size, $N_s = n_s/\ell^2 = \text{const}$, where n_s is the number of functioning sources per crystal.

Typical inputs for calculating plastic flow and energy dissipation rates of the organic crystalline explosives RDX and HMX are as follows: Let $\delta \approx d = b =$ one lattice spacing $\approx 5\times10^{-10}$ m, $W_0 = d/10$, and $\beta = 1$. For simplicity, assume that there is always sufficient energy to create new dislocations so that $p_c = 1$, and consequently, $d\gamma/dt = d\gamma/dt|_{\max}$. For the source size, let $\ell_s = 5\times10^{-7}$ m and assume that there is one functioning source per 5×10^{-6} m of crystal so that $N_s\ell = n_s/\ell = 2\times10^5$ sources per m of crystal. Let $v_0 = 2\times10^3$ m/s and $U_0 = (V/2G)\tau_Y^2$ where τ_Y is the macroscopic yield stress, $\tau_Y \approx 10-20$ MPa. G is the shear modulus, $G_{\mathrm{RDX}} \approx 4$ GPa, $G_{\mathrm{HMX}} \approx 4.5$ GPa. For the volume of the dislocation core let $V \approx \pi(2d)^2 d$, where the effective radius of the dislocation core is taken as $2d$. Following Gilman,[39] the mass m of the dislocation is approximately ρV, where ρ is the crystalline density which for a typical explosive $\approx 1.8\times10^3$ kg/m^3 so that $m \approx 2.83\times10^{-24}$ kg. Finally, we approximate the damage term as $(dU_0/dx)(\delta dN)/\ell \approx U_0\ell_d/\ell$ where ℓ_d is the damage length. This allows the distorted lattice potential to be simplified as $U = U_0(1+\ell_d/\ell)$. For these calculations let $\ell_d = 2\times10^{-6}$ m.

---

[1] J. Sharma and C. S. Coffey, in *Shock Compression of Condensed Matter*, edited by S. C. Schmidt and W. C. Tao (AIP Press, Woodbury, NY, 1995), p. 811.

[2] J. Sharma, and C. S. Coffey, in *Decomposition, Combustion, and Detonation Chemistry of Energetic Materials*, edited by T. B. Brill, T. P. Russell, W. C. Tao, and R. B. Wardle, MRS Symposia Proceedings No. 418 (Materials Research Society, Pittsburgh, 1995), p. 257.

[3] J. Sharma and C. S. Coffey (unpublished).

[4] C. Kittel, *Introduction to Solid State Physics*, 3rd ed. (Wiley, New York, 1968).

[5] U. F. Kocks, A. S. Argon, and M. F. Ashby, in *Progress in Material Science*, edited by B. Chalmers, J. W. Christian, and T. B. Massalski (Pergamon Press, New York, 1975).

[6] A. V. Granato, K. Lucke, J. Schlipf, and L. J. Teutonico, J. Appl. Phys. **35**, 2732 (1964).

[7] W. G. Johnston and J. J. Gilman, J. Appl. Phys. **30**, 129 (1959).

[8] Typically, $v_0 \approx 2$ to 5 km/s and the lattice spacing $d \approx 2$ to 5×10^{-10} m, so that the time for a dislocation with velocity v_0 to move one lattice spacing is $\approx 10^{-13}$ s.

[9] N. W. Ashcroft and N. D. Mermin, in *Solid State Physics* (Saunders, Philadelphia, 1976); see the deBoer analysis, p. 412.

[10] C. S. Coffey, Phys. Rev. B **49**, 208 (1994).

[11] C. S. Coffey, in *Mechanics of Deformation at High Rates*, edited by R. Graham (Springer-Verlag, Berlin, 1996), Vol. 3.

[12] A. Messiah, in *Quantum Mechanics* (North-Holland, Amsterdam, 1962), Vol. 1.

[13] C. S. Coffey, J. Appl. Phys. **70**, 4248 (1991).

[14] E. Z. Orowan, Z. Phys. **89**, 605 (1934); **89**, 634 (1934).

[15] C. S. Coffey, Phys. Rev. B **24**, 6984 (1981).

[16] C. S. Coffey, Phys. Rev. B **32**, 5335 (1984).

[17] D. Dlott and M. Fayer, J. Phys. Chem. **97**, 1901 (1993).

[18] S. A. Sheffield and D. D. Bloomquist, 7th Symposium on Detonation, Office of Naval Research, Arlington, VA, Report No. 82-334, 1982, p. 1084.

[19] E. O. Hall, Proc. Phys. Soc. London, Sect. B **64**, 747 (1951).

[20] N. J. Petch, J. Iron Steel Inst., London **174**, 25 (1953).

[21] J. D. Campbell and W. G. Ferguson, Philos. Mag. **21**, 63 (1970).

[22] P. S. Follansbee, G. Reggazzoni, and U. F. Kocks, in *Mechanical Properties at High Rates of Strain*, Institute of Physics Conference No. 70, edited by J. Harding (Institute of Physics, London, 1984).

[23] D. Price, in *Proceedings of the 5th Symposium on Detonation* (Office of Naval Research, Arlington, VA, ACR-184, 1970), p. 207.

[24] R. J. Spear and V. Nanut, in *Proceedings of the 9th Symposium on Detonation* (Office of Naval Research, Arlington, VA, 1989), p. 98.

[25] A. M. Frank, in Lawrence Livermore National Laboratory Report No. UCRL-LR-109534-92-2, Livermore, CA, 1992.

[26] J. Roth, in *Encyclopedia of Explosives and Related Items*, edited by S. M. Kaye, Picatinny Arsenal Report No. 2700, Picatinny Arsenal, Dover, NJ, 1980, Vol. 9, p. S 58.

[27] C. S. Coffey and V. F. DeVost, Propellants, Explos., Pyrotech. **20**, 105 (1995).

[28] dE/dt has units of J/s per meter of dislocation length J/(sm).

[29] I. Plaskin (unpublished).

[30] H. Moulard, in *Proceedings of the 9th Symposium on Detonation* (Office of Naval Research, Arlington, VA, 1989), Vol. I, p. 18.

[31] Detonation threshold pressures were determined in the heavy walled steel cylinder of the NOL Large Scale Gap Test. I. Jaffe, R. Beauregard, and A. Amster, in *Proceedings of the 3rd Symposium on Detonation* (Office of Naval Research, Arlington, VA, 1960), p. 584.

[32] C. S. Coffey, in *Decomposition, Combustion, and Detonation Chemistry of Energetic Materials*, edited by T. B. Brill, T. P.

Russell, W. C. Tao, and R. B. Wardle, MRS Symposia Proceedings No. 418 (Materials Research Society, Pittsburgh, 1995), p. 331. Here it was shown that the shear stress in a crystal is $\tau = \text{grad } P \cdot dr$ and for a cylindrical geometry $P(r) = P_0 e^{\alpha z} J_0(\alpha r)$. Since the cylindrical geometry is fixed in these gap tests the pressure and shear stress amplitudes required to initiate detonation are related, $P_{\text{cal}} = P_{\text{ref}} \tau_{\text{cal}} / \tau_{\text{ref}}$.

[33] PBXN-110 contains 66% 300 μ HMX 22% 40 μ HMX and 12% HTPB (hydroxyl terminated polybutadiene) binder. PBXN-128 is 77% 5 μ HMX and 23% HTPB binder. EXP-3 is 56% 5 μ HMX, 28% 132 μ NTO and 16% HTPB binder. EXP-4 is 56% 4 μ HMX, 28% 132 μ NTO and 16% HTPB binder. Here the insensitive explosive NTO ($C_2H_2N_4O_3$) was treated as an inert. The above scaling relation is used to avoid the problems of accounting for the binder and the binder-crystal interface.

[34] The inputs used to calculate the 1 μ HMX particle size initiation shear stress lie on the edge of what should be appropriate. Better input data are currently not available.

[35] These detonation threshold pressures were determined by a set of shock tests, which allows the simple scaling relation given in Ref. 31 to be used to relate the calculated shear stress for detonation initiation with the observed detonation threshold pressure.

[36] P. J. Herley, P. W. M. Jacobs, and P. W. Levy, J. Chem. Soc. A **3**, 434 (1971).

[37] P. J. Coyne, W. L. Elban, and M. A. Chiarito (unpublished).

[38] To estimate the temperature increase during impact assume the minimum dislocation number density $N = 10^{10}$ dislocations/m^2, so that $dE/dt \approx 10^{-1}$ J/s per meter of dislocation length. Assume that this energy is thermalized in a volume 100 molecular spacings in diameter and of unit length and that the explosive has a density of 1.8×10^3 kg/m^3. Assume also a typical energy dissipation time for impact $\approx 5\times 10^{-6}$ s and a specific heat of $C_v \approx 1.3\times 10^3$ J/(kg s) so that $\Delta\Theta \geqslant 300$ K.

[39] J. J. Gilman (private communication).