Modeling ratchet growth as porosity creep

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Abstract— Irreversible thermal cycling growth (or ratchet growth) of insensitive explosive formulations has been known for years. Traditionally it's attributed to material texture and to anisotropic thermal expansion. Although this understanding has been accepted for a long time, we're not aware of any model on the macroscale that connects these material properties to ratchet growth behavior. Thompson et al. [1] have observed that they get growth not just from thermal cycling, but also from a long hold time of the material sample at high temperature, and that such growth resembles creep response. Following their findings we propose here a predictive model for ratchet growth on the macroscale, where we assume that when temperature is increased, growth comes about by porosity (or volume) creep. As is well known, PBXs are prepared by die or isostatic pressing, and at the end of such pressing the material is left at porosity of about 2%, and with substantial residual or internal stress fluctuations in self-equilibrium. We model ratchet growth by assuming that: 1) increasing temperature decreases strength in tension (negative pressure), causing the porosity in the part of the material (in a control volume) that is in tension to creep (slowly increase); and 2) increasing temperature increases the internal pressure/tension fluctuations because of thermal expansion anisotropy, thereby enhancing the rate of porosity creep and ratchet growth. We write down equations for porosity creep and the resulting ratchet growth, and we demonstrate that our modeled ratchet growth results are similar to test data. We do not calibrate the free parameters of our model to reproduce specific data, as we do not own such data.

Keywords— creep, thermal cycling growth, ratchet growth.

I. INTRODUCTION

The phenomenon of growth (porosity and volume increase) as a result of thermal cycling of insensitive explosive formulations has been known for more than 30 years. Ratchet growth response increases sensitivity and causes safety concerns, and this is why it has been thoroughly studied [1-6]. Since the first studies of ratchet growth it has been assumed that it is related to material texture and anisotropic thermal expansion. But this assumption has not been verified, and we're not aware that any mechanism or model has been proposed to connect material anisotropy to ratchet growth data directly.

Progress towards understanding the mechanism of ratchet growth was made by observations of Thompson et al. in [1]. They performed tests in which they extended the hold time at high temperature. In these tests they observed that: 1) volume (or porosity) grows even at a constant high temperature, and not just during thermal cycling; and 2) the volume growth pattern is similar to what one gets from creep tests. From these results they concluded that ratchet growth is a creep-like phenomenon. In addition, we've wondered if ratchet growth is specific only to insensitive explosive formulations. Searching the literature extensively, we haven't found until recently any study looking for ratchet growth of any other explosive formulation. But recently we bumped upon such a report from people working on the development of insensitive munitions (IM) [7]. As IM contain insensitive explosive formulations, it makes sense that their developers would be concerned with ratchet growth. Accordingly, it turns out that thermal cycling is a standard test for IM development. In [7] they report the results of their standard thermal cycling test on various formulations of the explosives: RDX, HMX, NQ, AP, and DNAN, for which they find substantial amounts of ratchet growth (between 3 and 15%). Their goal is to develop formulations with less than 1% ratchet growth in their standard test.

In what follows we propose a macroscale model for ratchet growth, based on the assumption that growth at high temperature comes about by porosity (or volume) creep.

II. MODEL DESCRIPTION

Plastic bonded explosives (PBX) are manufactured by die or isostatic pressing of small explosive grains covered with a thin layer of plastic binder. The resulting material is inhomogeneous on the mesoscale with about 2% porosity. For isostatic pressing the pressure is about 200MPa at a temperature of about 100^0C, far from the pressure needed for full pore closure.

Accordingly we assume that after pressure removal and cooling to room temperature, the pressed material contains residual stresses (mainly pressure) in self-equilibrium. We're not aware that this has been quantitatively studied and documented. But it's not unreasonable to assume that because of the inhomogeneity of the material on the mesoscale (grain scale), such self-equilibrated residual stresses would form. With nowadays modeling capabilities such residual stresses can be computationally predicted with satisfactory accuracy. For simplicity we neglect here the shear residual stresses on the macroscale, and concentrate on the isotropic (pressure) residual stresses. Because of the low shear strength of the binder, the overall shear strength is quite small, and we assume that macroscopic residual shear stresses on the macroscale can be neglected compared to the macroscopic residual isotropic stresses. This assumption can (and should) be checked by simulation of the pressing process on the mesoscale. Again for simplicity, we further assume that in every macroscopic control volume (or macroscopic computational cell), half the mass is in compression with pressure P_c, and the other half is in tension (negative pressure) with pressure P_t. As the residual stresses are in self-equilibrium, we have: $P_c + P_t = 0$. We also assume that the material has porosity (or volume) strength on the macroscale, which is different for compression and tension. We denote these strength values by Z_{mc} and Z_{mt} for compression and tension, respectively. Volume strength on the macroscale results from shear strength on the mesoscale, and it is intuitively obvious that shear strength on the mesoscale in tension would be much smaller that shear strength on the mesoscale in compression. This is because plastic flow on the mesoscale in compression requires fracture and flow of the grains, while plastic flow on the mesoscale in tension requires

mainly tensile and shear deformation of the binder and grain separation. We therefore assume that $Z_{mc} >> Z_{mt}$, which can be verified and quantified as well by computer simulations on the mesoscale.

From these assumptions it would follow that porosity creep (and therefore also ratchet growth) may result from temperature increase, because porosity (or volume) strength in tension on the macroscale decreases as temperature increases. Accordingly, porosity (or volume) creep may result from temperature increase by the following steps: 1) initially (after a long stay at a constant temperature, say room temperature), the amount of tension is equal to the strength in tension, $P_{mt} = Z_{mt}$; 2) raising the temperature, Z_{mt} decreases and porosity (or volume) creep begins. As a result, porosity increases, volume increases (density decreases), and tension decreases. At the same time pressure (in absolute value) also decreases, as pressure and tension are self-equilibrated; 3) when temperature goes back to its initial value (thermal cycling), Z_{mt} increases back to its initial value, and porosity creep stops, but P_{mt} is now lower than initially; 4) for each additional thermal cycle, creep rate (and also volume growth rate) decreases according to the reduced distance between P_{mt} and Z_{mt}, and it finally decreases asymptotically to zero.

With this sequence of events we don't take into account the possible increase of P_{mt} with temperature as a result of anisotropic thermal expansion. We imagine that such an increase would happen irreversibly only on the first thermal cycle. If such an increase of P_{mt} does not happen, creep rate would stop before returning back to the initial temperature, and would be zero during the hold time at the initial temperature. Otherwise we would get a non-zero creep rate when holding at the initial temperature for some cycles. In the computed examples presented later we don't take into account the feature of anisotropic thermal expansion. In the next section we write down the equations for porosity (or volume) creep.

III. POROSITY (OR VOLUME) CREEP EQUATIONS

On the macroscale the material includes the matrix (m) (explosive grains and binder) and the voids (v). Specific volume V is given by:

$$V = V_m + V_v \quad \therefore \ V_m = V(1-\varphi) \quad for \quad \varphi = V_v/V$$

$$(1)$$

where φ=porosity. Time differentiating the first equation of (1) we get:

$$\dot{V}/V = \dot{V}_m/V + \dot{V}_v/V \quad \dot{\varepsilon} = \dot{V}/V \quad \dot{\varepsilon}_m = \dot{V}_m/V_m$$

$$\therefore \dot{\varepsilon} = \dot{\varepsilon}_m(1-\varphi) + \dot{\varepsilon}\varphi + \dot{\varphi} \quad \therefore \dot{\varepsilon} = \dot{\varepsilon}_m + \frac{\dot{\varphi}}{1-\varphi} \quad (2)$$

where volume strain (ε) and pressure (see later) are positive in tension. As explained above, we assume that for each computational cell half the cell is in tension and the other half in compression, and that the two halves differ in terms of porosity and specific volume. We index variables in the tension half by t and variables in the compression half by c. The last equation of (2) in the two halves is then:

$$\dot{\varepsilon}_t = \dot{\varepsilon}_{mt} + \frac{\dot{\varphi}_t}{1-\varphi_t} \quad \dot{\varepsilon}_c = \dot{\varepsilon}_{mc} + \frac{\dot{\varphi}_c}{1-\varphi_c} \quad (3)$$

As explained above, we assume that Z_{mc} (see above) is quite high and the half in compression does not creep, so that $\dot{\varphi}_c = 0$. We also assume that Maxwell's mechanical model holds here and the two halves deform at the same rate, so that: $\dot{\varepsilon}_c = \dot{\varepsilon}_t = \dot{\varepsilon}$. It therefore follows from Eq. (3) that:

$$\dot{\varepsilon}_{mc} - \dot{\varepsilon}_{mt} = \frac{\dot{\varphi}_t}{1-\varphi_t} \quad (4)$$

As we deal here with slow deformation (caused by slow thermal changes), we may convert volume strain to pressure using the isothermal bulk modulus K. Multiplying Eq. (4) by K we get:

$$\dot{P}_{mc} - \dot{P}_{mt} = K\frac{\dot{\varphi}_t}{1-\varphi_t} \quad (5)$$

Applying Herrmann's assumption [8, 9] for porous materials: $P=P_m(1-\varphi)$ we get:

$$P_c = P_{mc}(1-\varphi_c) \quad \therefore \dot{P}_c = (1-\varphi_c)\dot{P}_{mc}$$

$$P_t = P_{mt}(1-\varphi_t) \quad \therefore \dot{P}_t = (1-\varphi_t)\dot{P}_{mt} - P_{mt}\dot{\varphi}_t \quad (6)$$

$$\therefore \frac{\dot{P}_c}{1-\varphi_c} - \frac{\dot{P}_t}{1-\varphi_t} = (K+P_{mt})\frac{\dot{\varphi}_t}{1-\varphi_t}$$

And using the self-equilibrium equation $\dot{P}_c + \dot{P}_t = 0$ we finally get:

$$\dot{p}_t\left(\frac{1}{1-\varphi_c} + \frac{1}{1-\varphi_t}\right) = -\left(K + \frac{P_t}{1-\varphi_t}\right)\frac{\dot{\varphi}_t}{1-\varphi_t} \quad (7)$$

Using our overstress approach for the rate of change of porosity [8], we assume that it increases with the overstress P_{mt}-Z_{mt}, and for the lack of any specific knowledge about this dependence, we assume for it a linear relation:

$$\dot{\varphi}_t = A_\varphi(P_{mt} - Z_{mt}) \quad \text{for} \quad P_{mt} > Z_{mt}$$

$$\dot{\varphi}_t = 0 \quad \text{for} \quad P_{mt} \leq Z_{mt} \quad (8)$$

where A_φ is a material parameter to be determined from tests.

It follows from Eq. (8) that **the key to porosity (or volume) creep (and therefore to ratchet growth) is the decrease of Z_{mt} with temperature.**

We assume for this decrease the following linear relation:

$$\dot{Z}_{mt} = -\frac{Z_{mt0}}{T_{melt} - T_0}\dot{T} \quad \text{for} \quad T < T_{melt}$$

$$\dot{Z}_{mt} = Z_{mt} = 0 \quad \text{for} \quad T \geq T_{melt} \quad (9)$$

where T_0=room temperature, and Z_{mt0}=volume strength in tension at T_0. We define growth (=g) as g=ε-ε_0. Assuming that ε_0=0 and using Eqs. (3) and (6) we get:

$$\dot{g} = \dot{\varepsilon}_{mt} + \frac{\dot{\varphi}_t}{1-\varphi_t} = \frac{\dot{P}_{mt}}{K} + \frac{\dot{\varphi}_t}{1-\varphi_t}$$

$$\dot{P}_{mt} = \frac{\dot{P}_t}{1-\varphi_t} + P_t\frac{\dot{\varphi}_t}{(1-\varphi_t)^2} \quad (10)$$

It can be seen from the above equations that we get a system of 5 time dependent ODEs with the following unknowns: temperature T, tensile-half porosity φ_t, tensile-half volume strength Z_{mt}, tensile-half isotropic tensile stress P_t and growth or volume strain increase g. We integrate this system of 5 ODEs with a standard Runge-Kutta 4th order solver with constant time steps Δt. We use Δt=1sec.

IV. COMPUTED EXAMPLES

We use the following parameters: bulk modulus K=3500MPa, initial volume strength Z_{m0}=100MPa (of the

order of isostatic pressing pressure), initial porosity φ_0=2%, porosity rate of increase coefficient A_φ=1.e-7/sec/MPa, initial temperature 23^0C, [1], final temperature 113^0C, as in [1], ramp temperature increase and decrease time 1.5 hours, and hold time at low and high temperature 1 hour.

In Fig. 1 we show results for a run with a single thermal cycle. We see (in red) the outline of the thermal cycle and (in blue) the growth (volume strain increase) with time. We see that growth increases until sometime after the start of temperature drop, and then it stays unchanged as Z_{mt} goes above P_{mt}. We also see that the maximum growth is about 0.5%, similar to what they got in [1].

Fig.2: Growth from a run with a long hold time at the high temperature.

Fig.1: Growth from a run with a single thermal cycle.

In Fig. 2 we show results from a run in which we hold the high temperature for a long time. We do that by increasing the high temperature hold time to 10 hours. We see from Fig. 2 that when the hold time at the high temperature is high, growth continues to about 0.7%, as suggested in [1]. Next we check the influence of the coefficient of porosity increase rate A_φ (Fig. 3) and of the isothermal bulk modulus K (Fig. 4). Both are for a single thermal cycle as in Fig. 1. Finally we show in Fig. 5 the results of a run of 15 cycles. For this run we changed the hold time at the low temperature to 10 minutes, as in the tests reported in [2]. We see in Fig. 5 that as before, the full growth history has flat sections at and near the low temperature. Following [2] we also show growth values at the end of each of the thermal cycles (blue dots). A curve through these dots seems continuous, as in [2].

Fig.3: Influence of the coefficient A_φ on growth for a single thermal cycle as in Fig. 1.

Fig.4: Influence of the isothermal bulk modulus K on growth for a single thermal cycle as in Fig. 1.
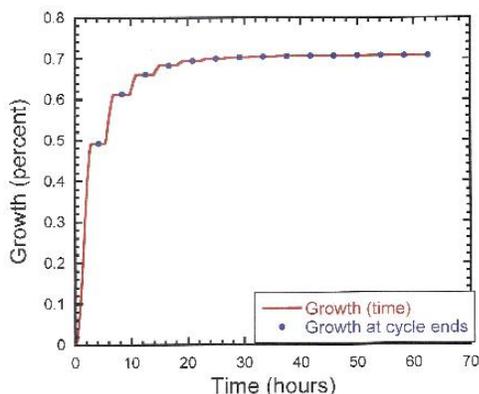
Fig.5: Ratchet growth history for 15 thermal cycles. Red: continuous growth history.

Blue: growth at the end of each cycle.

V.   SUMMARY

Early on it was suggested that ratchet growth results from texture of the explosive crystals and from anisotropy of its thermal expansion. But as far as we know, this suggestion has not led to a model that can predict ratchet growth response on the macroscale. In [1] they observed that: 1) growth occurs not just from thermal cycling, but also for a long hold time at a high temperature; and 2) the overall growth behavior is creep-like. Here we build on these observations and develop a predictive ratchet growth model on the macroscale. We assume that: 1) after pressing, the material has residual stresses on the mesoscale that are self-equilibrated on the macroscale; 2) shear stresses on the macroscale can be neglected, and what causes growth is porosity (or volume) creep (slow porosity increase) in the tension part of the isotropic stress; and 3) as temperature is raised, the volume strength (resistance to porosity creep) on the tension part decreases, and the tension part creeps Based on these assumptions we write down equations for ratchet growth on the macroscale. The equations include only a single parameter to be calibrated from tests, which is the coefficient of the overstress porosity growth rate equation. We show results of ratchet growth computations which look similar enough to test data.

REFERENCES

[1] D.G. Thompson, R.B. Ashwarz, G.W. Brown and R. DeLuca, Time-evolution of TATB based irreversible thermal expansion (ratchet growth), Propellants, Explos. Pyrotech, 40, 558-565 (2015).

[2] D.G. Thompson, R.B. Ashwarz and R. DeLuca, Irreversible volume expansion of a TATB based composition, SCCM AIP Conf. Proc. 1793, 040003, 1-4 (2015).

[3] C.S. Waznick, G.G. Thompson, R. DeLuca, B.M. Patterson and T.A. Shear, Thermal cycling and ratchet growth of as pressed TATB pellets, SCCM AIP Conf. Proc. 1979, 060011, 1-5 (2017).

[4] D.G. Thompson, G.W. Brown, B. Olinger, J.T. Mang, R. DeLuca and S. Hagelberg, The effects of TATB ratchet growth on PBX 9502, Propellants, Explos. Pyrotech. 35,507-513 (2010).

[5] R.H. Gee, A. Maiti and L.E. Fried, Mesoscale modeling of irreversible volume growth in powders of anisotropic crystals, Appl. Phys. Letters 90. 254105 (2007).

[6] R.N. Mulford and J.A. Romero, Sensitivity of the TATB based explosive PBX 9502 after thermal expansion, CP429, ACCM, 723-726 (1997).

[7] P. Samuels, Irreversible growth of DNAN based formulations, RDECOM, NDIA IM/EM, Las Vegas, NV (2012).

[8] W. Herrmann, Constitutive equation for the dynamic compaction of ductile porous materials, J. Appl. Phys. 40, 2490-2499 (1969).

[9] Y. Partom, Modeling dynamic gradual and rate dependent closing and opening of pores in porous materials, Shock Compression of Condensed Matter conference, St. Louis MO (2017).