LA-UR- 09-05524

Approved for public release; distribution is unlimited.

Title:	CONSTITUTIVE MODELING OF SHOCK RESPONSE OF PTFE
Author(s):	Anatoly D. Resnyansky, Neil K. Bourne, Jeremy C.F. Millett, Eric N. Brown
Intended for:	APS SCCM

Los Alamos
NATIONAL LABORATORY
EST. 1943

Form 836 (7/06)

CONSTITUTIVE MODELING OF SHOCK RESPONSE OF PTFE

A. D. Resnyansky[1], N. K. Bourne[2], J. C. F. Millett[2], and E. N. Brown[3]

[1]Weapons Systems Division, DSTO, Edinburgh SA 5111, Australia
[2]AWE, Aldermaston, Reading, RG7 4PR, Berkshire, UK
[3]Los Alamos National Laboratory, ADWP MS A-113, Los Alamos, NM 87545, USA

Abstract. The PTFE (polytetrafluoroethylene) material is complex and attracts attention of the shock physics researchers because it has amorphous and crystalline components. In turn, the crystalline component has four known phases with the high pressure transition to phase III. At the same time, as has been recently studied using spectrometry, the crystalline region is growing with load. Stress and velocity shock-wave profiles acquired recently with embedded gauges demonstrate features that may be related to impedance mismatches between the regions subjected to some transitions resulting in density and modulus variations. We consider the above mentioned amorphous-to-crystalline transition and the high pressure Phase II-to-III transitions as possible candidates for the analysis. The present work utilizes a multi-phase rate sensitive model to describe shock response of the PTFE material. One-dimensional experimental shock wave profiles are compared with calculated profiles with the kinetics describing the transitions. The objective of this study is to understand the role of the various transitions in the shock response of PTFE.

Keywords: Constitutive modeling, phase transition; shock wave, multi-phase material.
PACS: 47.40.Nm, 62.50.Ef, 64.70.km.

INTRODUCTION

PTFE is a complex material with four known phases conventionally locating their states in the pressure-temperature space. The amorphous component is typically observed at any state of the bulk material. However, three crystalline phases characterized by molecule twisting, namely, II, IV, and I are progressively evolving into less twisted modifications, respectively, with temperature increase. In addition, the crystalline phases are transforming into a planar modification (phase III) when pressure increases. However, the transitions, specifically the high-pressure one, may be affected by other parameters such as the stress deviator (martensitic transition) as mentioned in [1] and time, manifesting the kinetic nature of the transitions, as observed in [2]. When treating PTFE as a composite with amorphous and a crystalline phase that can be a relatively soft one (phase I) or a harder phase II, the Taylor tests [3] have demonstrated that possible inclusions of a harder crystalline phase (such as the phase III) or even increase in crystallinity can be a reason of the brittleness increase of the PTFE rods impacting anvil. Therefore, the present paper is an attempt to consider constitutive effects within shock waves using a multi-phase model for experimental data [4] on velocity profiles in PTFE at two velocity impacts with presumably dominating phases II and III, respectively.

MODEL

The present model simplifies the material as a three-phase mixture of the phases that may have

strength. The phases are in the velocity equilibrium between them, whereas all other parameters can be specific to the phases. The model prototype for a material without strength has been published in [5] with an earlier version ignoring the inter-phase heat transition effects in [6]. The strength effects are coped with in the manner suggested for a model published in [7]. The resulting thermodynamically consistent system of equations included the mass, momentum and energy conservation laws in a conventional form similar to [7] and constitutive equations for the mass concentrations c_2 and c_3 for second and third phase specified for the model (concentration for first phase is complimentary: $c_1=1-c_2-c_3$), and, similarly, equations for the volume concentrations θ_2 and θ_3. These equations are used in the manner suggested in [5-6]. Initially, $c_2=0.472$ and $c_3=0.52$. Thermal non-equilibrium is considered similarly to [6] for corresponding thermal non-equilibrium parameters χ_2 and χ_3. Two additional constitutive parameters λ_2 and λ_3 are associated with possible inter-phase strain deviatoric non-equilibrium. The multi-phase decoupled shear strain component e_1 for the one-dimensional case in the model [7] is considered in a manner similar to the analysis [8]. Constitutive equation for an effective strain for the multi-phase mixture is introduced in the manner [7]. Conventional materials of experimental assemblies are described with the model [9] realized in the form [7]. The system of equations is closed by equations of state for the conventional materials and phases of PTFE in the form used in [5-7] and parameters of constitutive equations are selected in the way described in [5], using two yield stress points versus two strain rates. The yield stress data for PMMA were taken from [10] and for PTFE from [11]. The yield stress is considered to be balanced between the PTFE phases. Elastic constants for the PTFE material were taken from [11] and allocated between the phases using considerations [12] as a guidance.

The first and second phases have similar characteristics in the present work. For the first phase, representing the amorphous phase, density $\rho_0 = 2.04 g/cm^3$, shear and bulk modulus are G = 0.034 GPa, and K=0.57 GPa, the thermal capacity $c_V = 2$ J/(g·grad), and the Gruneisen coefficient is 0.95. The compressibility coefficients are from a rough correlation with Hugoniots. For the second phase, representing a soft crystalline phase, density $\rho_0=2.3 g/cm^3$, shear and bulk modulus are G=0.068 GPa and K=1.13 GPa, the thermal capacity $c_V=1.5$J/(g·grad), and the Gruneisen coefficient is 0.9. For the third phase, representing a hard crystalline phase, density $\rho_0= 2.355$ g/cm^3, shear and bulk modulus are G=1.186 GPa and K=3.35 GPa, the thermal capacity $c_V =1$ J/(g·grad) and the Gruneisen coefficient is 0.3.

The transition kinetics is representing a transformation of the first phase into the third phase, which is initiated at the pressure above the line in the (p,T)-phase diagram corresponding to the transition from Phase II into Phase III. In the present work it is approximated by the critical pressure at 0.65GPa.

The model is coded with the Godunov method, using a technique described elsewhere [5].

RESULTS AND DISCUSSION

Velocity profiles obtained in [4] at high velocity impact of PTFE samples by PMMA flyer plates are analyzed below with the present model.

Two impact velocities 450 (Test A) and 850 m/s (Test B) for flyer plates of 2.5 and 5 mm thickness, respectively, were considered when impacting 20mm-thickness PTFE target. Attempts to describe the experiment of Test A with a conventional model provide reasonable results with the velocity reached at the flyer-target interface controlled mainly by the impedance match, shown in Fig. 1. The calculated velocity profiles are taken at the velocity gauge locations at 1, 3, 5, and 7 mm in the target in accordance with the set-up [4] and marked by numbers 1 to 4, respectively. Similarly to [4], the profiles are normalized to $\tau_0=5$ and 3 μsec with correspondingly stretched experimental records for Tests A and B, respectively. The particle velocity mismatch of calculation with experiment is due to the lack of information about the modulus and compressibility of specified phases. Evolution of the upper portion (above 300 m/s) of calculated profiles for Test B is shown in Fig. 1 by curves 1'-4'. Thus, without accounting for the phase transition, at a higher impact velocity the release effects attenuate the pulse very quickly (shown in Fig. 2). This contradicts with the results of [4] where the velocity plateau is very similar to that for the low-velocity test as shown with an

upper portion of the experimental records for Test B. This apparent shock attenuation feature is possibly associated with the phase transition effects. The phase transition can be associated with transformation either from a soft (from the elastic modulus viewpoint) crystalline phase into a hard one or from an amorphous phase into a hard crystalline phase. Unfortunately, the experiments and the modeling cannot differentiate these types of transformations. Therefore, the transition, we analyze, can be associated with either.

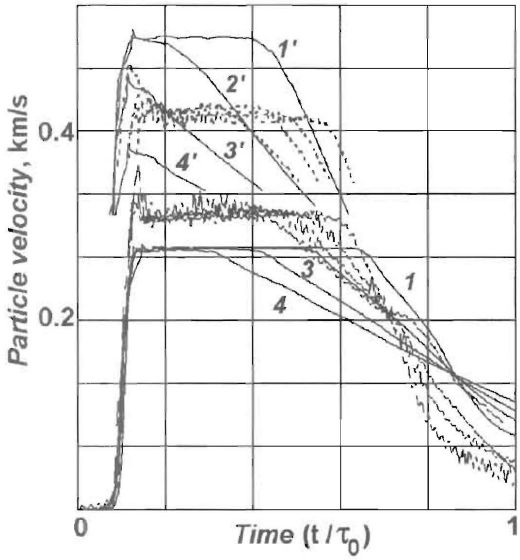

FIGURE 1. The calculated velocity profiles compared with experiment (dashed) curves for the Test A (1-4) and Test B (1'-4') without the phase transition.

A distinctive precursor, in case if pressure and temperature are the only parameters controlling the transition, is not observed in the experimental velocity profiles. Therefore, it is natural to suggest that the most noticeable phase transition effects can be observed in the release wave, as noted in [4]. One of the most significant effects on the load mode of the material is the shearing that results from the change of the shear direction into an opposite one when the release wave overtakes the shock wave. At the same time, a very quick transition in the shock front might be possible with an effect on the particle velocity level at the plateau. However, in the present work we focus on possible effects in the release wave. Therefore, we have aimed at simulation of a martensitic transition when conditions of the Phase II to Phase III transition are satisfied (the x-stress is above the critical pressure value of 0.65 GPa). Therefore, the mass concentration of a hard phase (the third phase) was allowed to grow from the first phase when the pressure exceeds the critical line p=0.65 GPa. The growth rate was controlled by a relaxation parameter in the equation for c_3, which is proportional to the stress deviator when it agrees with the stress deviator sign in the release wave.

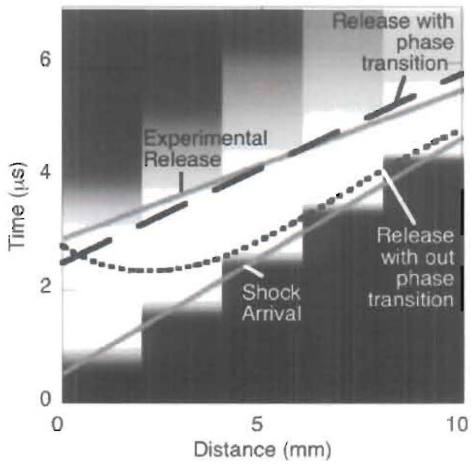

FIGURE 2. Lagrangian distance-time plot for Test B of calculated release with and without martensitic phase transition compared with experiment. The gray scales run from black to white for the experimental data [4], with white the maximum particle.

The calculation results are shown in Fig. 3. Analysis of the wave interaction during the calculation indicates that the plateau is a result of interaction between the rarefaction wave from the rear side of the flyer plate with a part of material in the vicinity of the impactor-target interface that is hardening during the phase transition because of the crystallinity increase or the Phase II-III transition (or both). Thus, the hardened area serves as a hard expanding piston separating the flyer plate from the remaining target As a result, the rarefaction process in the flyer plates takes a smaller effect on the pulse. As shown in Fig. 2, inclusion of the martensitic phase transition

captures the release response observed experimentally.

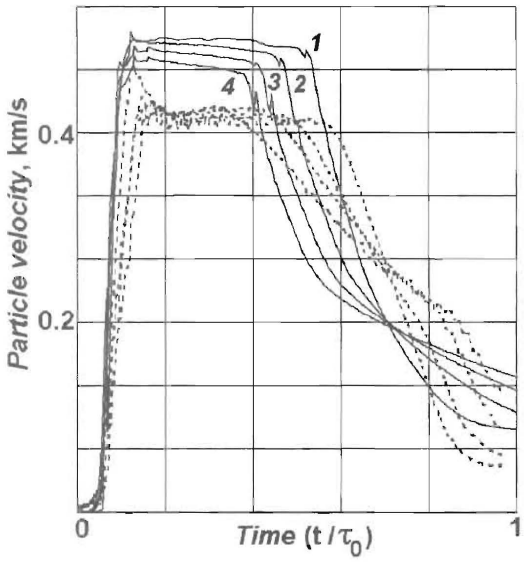

FIGURE 3. The calculated velocity profiles compared with experiment [4] for Test B with the phase transition kinetic of martensitic type.

DISCUSSION AND CONCLUSIONS

The modeling has demonstrated that the release effects of experimental velocity profiles in PTFE above the high pressure transition line may be associated with a martensitic transformation.

In order to identify whether the crystallinity rise of the change of crystalline phases is actually a reason for the observed feature, mechanical properties of the amorphous phase and specific crystalline phases should be yet specified.

The particle velocity mismatch between the calculated and experimental values may be associated either with the phase properties yet to be determined or with an additional (non-martensitic) very quick transformation of the II-to-III type occurring at the head of the shock front and reducing the velocity behind the front.

REFERENCES

1. E.N. Brown, D.M. Dattelbaum, D.W. Brown, P.J. Rae, B. Clausen, A new strain path to inducing phase transitions in semi-crystalline polymers, Polymer, 2007, 48(9), 2531-2536.
2. E.N. Brown, C.P. Trujillo, G.T. Gray III, P.J. Rae, N.K. Bourne, Soft-recovery of polytetrafluoroethylene shocked through the crystalline phase II-III transition, J. Appl. Physics, 2007, 101(2), 024916.
3. P.J. Rae, G.T. Gray, D.M. Dattelbaum, N.K. Bourne, "The Taylor impact response of PTFE (Teflon)", in Shock Compression of Condensed Matter, 2004 (M.D. Furnish, Y.M. Gupta, J.W. Forbes, eds.) pp. 671-674.
4. N.K. Bourne, E.N. Brown, J.C.F. Millett, G.T. Gray III, Shock, release and Taylor impact of the semicrystalline thermoplastic polytetrafluoroethylene, J. Appl. Physics, 2008, 103(7), 074902.
5. A.D. Resnyansky, Constitutive Modelling of Hugoniot for a Highly Porous Material, J. of Appl. Physics, 2008, 104(9), 093511-14.
6. A.D. Resnyansky and N.K. Bourne, Shock-wave compression of a porous material, J. of Appl. Physics, 2004, 95(4), 1760 - 1769.
7. A.D. Resnyansky, Thermodynamically Consistent Decoupled Shear-Volumetric Strain Model and CTH Implementation, DSTO report, DSTO-TR-2299, 2009.
8. A.D. Resnyansky, E.I. Romensky, and N.K. Bourne, Constitutive Modelling of Fracture Waves, J. Appl. Physics, 2003, 93(3), 1537-1545.
9. Godunov S.K. and Romenskii E.I., Elements of Continuum Mechanics and Conservation Laws, Kluwer Academic Publ., N.Y., 2003.
10. Blumenthal W.R., Cady C.M., Lopez M.F., Gray III, G.T., and Idar D.J., "Influence of temperature and strain rate on the compressive behavior of PMMA and polycarbonate polymers", in Shock Compression of Condensed Matter, 2001 (M.D. Furnish, N.N. Thadhani, Y. Horie, eds.), pp. 665-668.
11. E.N. Brown, P.J. Rae, G.T. Gray III, The influence of temperature and strain rate on the tensile and compressive constitutive response of four fluoropolymers, J. de Physique IV, 2006, 134, 935-940.
12. E.N. Brown, P.J. Rae, D.M. Dattelbaum, B. Clausen, D.W. Brown, In-situ measurement of crystalline lattice strains in polytetrafluoroethylene, Exp. Mechanics, 2008, 48 (1), 119-131.