An Equation of State for Anisotropic Solids under Shock Loading

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An anisotropic equation of state is proposed for accurate extrapolation of high-pressure shock Hugoniot states to other thermodynamics states for shocked single crystals and polycrystalline alloys. The proposed equation of state represents mathematical and physical generalization of the Mie-Grüneisen equation of state for isotropic material and reduces to this equation in the limit of isotropy. Using an anisotropic nonlinear continuum framework and generalized decomposition of a stress tensor [A. A. Lukyanov, Int. J. Plasticity 24, 140 (2008)], the shock wave propagation along arbitrary directions in anisotropic solids of any symmetry can be examined. The non-associated strength model includes the distortion effect of the yield surface which can be used to describe the anisotropic strength differential effect. A numerical calculation showed that the general pulse shape, Hugoniot Elastic Limits (HELs), and Hugoniot stress levels for aluminum alloy 7010-T6 agree with the experimental data. The results are presented and discussed, and future studies are outlined.

INTRODUCTION

The shock waves and high-strain-rate phenomena are involved in many physical phenomena, therefore, we are interested in understanding the physical properties of solids under these non-trivial conditions. Investigation of different anisotropic solids (e.g., single crystals and polycrystalline alloys) under shock loading has found significant interest in the research community [1]-[10]. Modern, high-resolution methods to monitoring the stress and particle velocity histories in shock waves and equipment have been created [11], [15]; numerous investigations into the mechanical properties of different classes of materials have been undertaken [11], [19]-[28]; and numerous phenomenological as well as microscopic models have been developed [8], [11], [19], [29], [30]. However, in spite of a perfectly adequate general understanding, experimental methodology, and theory, material models do not agree in detail, especially for anisotropic solids. For many years, it has been assumed that the response of materials to shock loading is isotropic, and only recently has anisotropy in the shock response attracted the attention of researchers. In the early 2000s, Gray III et al. [6], [7] showed that under shock loading conditions (one-dimensional strain space), the variation of the Hugoniot elastic limit (HEL) or the yield strength of annealed zirconium was consistent with the quasi-static experimental data. To describe the anisotropic solids response under shock loading the following several factors must be addressed during the numerical modelling: (a) large compressions lead to a nonlinear behavior – an equation of state (EOS) is required, (b) low yield stresses lead to large plastic deformations – an appropriate strength model is required. To address these factors, thermodynamically consistent framework for modelling the response of single crystal and polycrystalline alloys under shock loading was developed. This framework, building on the thermodynamic approach of Wallace [1] and continuum framework of Johnson [2]-[3], couples nonlinear elasticity with non-associated anisotropic plasticity within a thermodynamically consistent numerical incremental formalism [3].

SHORTCOMINGS OF THE ISOTROPIC EQUATION OF STATE

The EOS for isotropic materials typically defines the pressure as a function of density \( \rho \) (or specific volume, \( \nu \)) and specific internal energy \( e \). Experimental shock Hugoniots have been widely used as reference state data for extrapolating to other high-pressure and high-temperature thermodynamic states. The extrapolation has been done by using a very popular form of equation of state that is used extensively for isotropic solid continua is the Mie-Grüneisen EOS:

\[
\Gamma (\nu) = \nu \left( \frac{\partial p}{\partial e} \right)_{\nu}, \quad \Gamma (\nu) = \frac{\gamma_0 + a \mu}{1 + \mu}, \tag{1}
\]

where \( \Gamma (\nu) \) is the Grüneisen gamma, \( \gamma_0 \) is the initial Grüneisen gamma, \( a \) is the first order volume correction to \( \gamma_0 \), and \( p \) is the hydrostatic pressure. Assuming \( \Gamma (\nu) \) to be a function of volume only [1], the Mie-Grüneisen EOS provides a simple extrapolation of a known set of Hugoniots data to other sets of thermodynamic states:

\[
p = f (\rho, e) = P_H \left( 1 - \frac{\Gamma}{2 \mu} \right) + \rho \Gamma e, \tag{2}
\]

where \( P_H \) is the Hugoniot pressure, \( \mu = \frac{\rho}{\rho_0} - 1 \) is the relative change of volume. The shock compression process is characterized by the Rankine-Hugoniot jump relations [11], [12], [29], [30]. The Rankine-Hugoniot equations for the shock jump conditions includes five variables: pressure \( p \), particle velocity \( u_p \), shock velocity \( U_s \), density \( \rho \) (or specific volume, \( \nu \)) and energy \( e \). Hence, an additional equation is needed. In many dynamic experiments, \( u_p \) (the particle velocity directly behind the shock) and \( U_s \) (the velocity at which the shock wave propagates
through the medium) are measured. The Hugoniot pressure and a shock velocity $U_s$ are a non-linear function of particle velocity $u_p$. Following Steinberg’s model [19], the shock velocity is:

$$U_s = c + S_1 u_p + S_2 \left( \frac{u_p}{U_s} \right) u_p + S_3 \left( \frac{u_p}{U_s} \right)^2 u_p, \quad (3)$$

where $c$ is the velocity curve intercept (can be approximated by the bulk speed of sound). Therefore, the Mic-Grüneisen equation of state with cubic shock velocity as a function of particle velocity defines pressure as

$$p = \frac{\rho_0 c^2 \mu \left[ 1 + \left( 1 - \frac{\mu}{\nu} \right) \mu - \frac{\mu^2}{2} \right]^2}{\left[ 1 - (S_1 - 1) \mu - S_2 \mu^2 - S_3 \frac{\mu^3}{(\mu + 1)} \right] + \left( 1 + \mu \right) \cdot \Gamma \cdot E}, \quad \mu > 0;$$

$$p = \frac{\rho_0 c^2 \mu + \left( 1 + \mu \right) \cdot \Gamma \cdot E}, \quad \mu < 0;$$

where $E$ is the internal energy per initial specific volume \( E = \frac{c}{\rho_0} \), $K$ is the classical bulk modulus, $S_1$, $S_2$, $S_3$ are the intercept of the $U-u_p$ curve. Parameters $c$, $S_1$, $S_2$, $S_3$, $\gamma_0$, $\alpha$ represent material properties which define its EOS. Parameters have been defined to cover a large number of isotropic materials [19].

**AN ANISOTROPIC EQUATION OF STATE**

Before discussing an anisotropic equation of state, the generalized decomposition of the stress tensor is summarized in [10]. The generalized decomposition framework will provide a useful point of construction an anisotropic equation of state.

**Generalized decomposition of the stress tensor: $\alpha$-$\beta$ decomposition**

The definition of pressure in the case of an anisotropic solids should be the result of stating that the "pressure" term should only produce a change of scale, i.e. isotropic state of strain. This should allow the calculation of the direct stress ratios that will produce only a change of scale [10]. The generalized decomposition of the stress tensor $\sigma_{ij}$ is defined as:

$$\bar{P} : \bar{S} = 0 \quad \text{or} \quad \alpha_{ij} \bar{S}_{ij} = 0, \quad \sigma_{ij} = p^* \alpha_{ij} + \bar{S}_{ij}, \quad (6)$$

where $\bar{P} = p^* \alpha_{ij}$ is the generalized spherical part of the stress tensor, $\bar{S} = \bar{S}_{ij}$ is the generalized deviatoric stress tensor, $p^*$ is the total generalized "pressure" and $\alpha_{ij}$ is the first generalization of the Kronecker’s delta symbol. The constructive definition of the tensor $\alpha_{ij}$ is based on the fact that stress tensor $\rho_{ij}$ is induced in the anisotropic medium by the applied isotropic strain tensor $\frac{\varepsilon}{3} \delta_{ij}$, i.e.

$$p_{ij} = -\frac{\varepsilon}{3} C_{ijkl} \delta_{kl}, \quad p = -K_C \varepsilon$$

where $p$ is the pressure, $\varepsilon$ is the volumetric strain, $\delta_{ij}$ is the Kronecker’s delta symbol (unit tensor), $C_{ijkl}$ is the elastic stiffness matrix, and $K_C$ is the first generalized bulk modulus. The expressions for $\alpha_{ij}$ and $K_C$ are presented at the end of Sect. Besides, everywhere contraction by repeating indexes is assumed. Using (6), the following expression for total generalized "pressure" $p^*$ can be obtained:

$$p^* = -\frac{\sigma_{ij} \alpha_{ij}}{\alpha_{kl} \alpha_{kl}} = -\frac{1}{\|\alpha\|^2} \sigma_{ij} \alpha_{ij},$$

where $\|\alpha\|^2 = \alpha_{ij} \alpha_{ij} = \alpha_{11}^2 + \alpha_{22}^2 + \alpha_{33}^2$, and finally, the expression for the generalized deviatoric part of the stress tensor can be rewritten in the following form:

$$\bar{S}_{ij} = \sigma_{ij} - \alpha_{ij} \cdot \frac{1}{\|\alpha\|^2} \sigma_{kl} \alpha_{kl}.$$  

For anisotropic materials, the total generalized "pressure" $p^*$ has been expressed [11] as:

$$p^* = p + \frac{\beta_{ij} \bar{S}_{ij}}{\beta_{kl} \alpha_{kl}}, \quad p = -\frac{\beta_{ij} \sigma_{ij}}{\beta_{ij} \alpha_{ij}},$$

where $p$ is the pressure related to the volumetric deformation $\varepsilon$ and $\beta_{ij}$ is the second generalization of the Kronecker’s delta symbol. The constructive definition of the tensor $\beta_{ij}$ is based on the fact that stress tensor $p\beta_{ij}$ is independent of the stress tensor $C_{ijkl} \varepsilon_{kl}$, i.e. their contraction product is zero for any deviatoric strain tensor $e_{kl}$, where $C_{ijkl}$ is the elastic stiffness matrix. The following relation describes the functional definition of the second order material tensor $\beta_{ij}$:

$$\beta_{ij} C_{ijkl} = 3 K_S \delta_{kl},$$

where $K_S$ represents the second generalized bulk modulus. The solution of equations (11) in terms of $\beta_{ij}$ components and expression for $K_S$ are presented below. Equa-tions (11) define the correct generalized "pressure" for the elastic regime. Note that the generalized decomposition of the stress tensor can be applied for all anisotropic solids of any symmetry and represents a mathematically consistent generalization of the conventional isotropic case. The procedure of construction for the tensor $\alpha_{kl}$ has been defined in [10]. The elements of the tensor $\alpha_{kl}$
are
\[
\alpha_{11} = \left( \sum_{k=1}^{3} C_{k1} \right) \cdot 3K_C, \quad \alpha_{22} = \left( \sum_{k=1}^{3} C_{k2} \right) \cdot 3K_C, \\
\alpha_{33} = \left( \sum_{k=1}^{3} C_{k3} \right) \cdot 3K_C, \quad \alpha_{ij} \alpha_{ij} = 3, \\
\text{(12)}
\]

\[
K_C = \frac{1}{3\sqrt{3}} \left[ \left( \sum_{k=1}^{3} C_{k1} \right)^2 + \left( \sum_{k=1}^{3} C_{k2} \right)^2 + \left( \sum_{k=1}^{3} C_{k3} \right)^2 \right],
\]

\[
K_S = \frac{1}{9K_C},
\]

where \(C_{ij}\) is the elastic stiffness matrix (written in Voigt notation). The elements of the tensor \(\beta_{kl}\) are
\[
\beta_{11} = \left( \sum_{k=1}^{3} J_{k1} \right) \cdot 3K_S, \quad \beta_{22} = \left( \sum_{k=1}^{3} J_{k2} \right) \cdot 3K_S, \\
\beta_{33} = \left( \sum_{k=1}^{3} J_{k3} \right) \cdot 3K_S, \quad \beta_{ij} \beta_{ij} = 3,
\]

\[
\frac{1}{K_S} = \sqrt{3} \left[ \left( \sum_{k=1}^{3} J_{k1} \right)^2 + \left( \sum_{k=1}^{3} J_{k2} \right)^2 + \left( \sum_{k=1}^{3} J_{k3} \right)^2 \right],
\]

(15)

where \(J_{ij}\) are elements of compliance matrix (written in Voigt notation). In the limit of isotropy, the proposed generalization returns to the traditional classical case where tensors \(\alpha_{ij}, \beta_{ij}\) equal \(\delta_{ij}\) and equations (10) take the form:
\[
p^* = -\frac{\sigma_{ij} \delta_{ij}}{\delta_{kl} \delta_{kl}}, \quad p = -\frac{\beta_{ij} \sigma_{ij}}{\delta_{kl} \alpha_{kl}} = -\frac{1}{3} \sigma_{kk},
\]

(16)

where \(p = -\frac{\sigma_{kk}}{3}\) is the classical hydrostatic pressure. Also, parameters \(K_C\) and \(K_S\) were considered as the first and the second generalized bulk moduli. In the limit of isotropy they reduce to the well-know expression for conventional bulk modulus.

**Thermodynamical framework**

During shock loading, the medium undergoes nonlinear behavior; therefore an equation of state (EOS) is required to describe the medium’s response under shock loading conditions. It is convenient for use in numerical codes to have an analytical form of the EOS. Such an analytic form is at best an approximation to the true relationship. Thermodynamical definition of the Grüneisen parameter \(\Gamma(\nu, T)\) is the following:
\[
\Gamma(\nu, T) = \frac{\nu}{C_\nu} \left( \frac{\partial S}{\partial \nu} \right)_T,
\]

(17)

where \(S\) is the entropy, \(T\) is the temperature, \(C_\nu\) is the heat capacity at constant specific volume. This definition may be generalized to a tensor \(\Gamma_{ij}\) for the stress-strain variables \([1]\):
\[
\Gamma_{ij} = \frac{\nu}{C_\nu} \left( \frac{\partial S}{\partial \varepsilon_{ij}} \right)_T,
\]

(18)

where \(\varepsilon_{ij}\) is the strain tensor and \(C_\nu\) is the heat capacity at constant strains. Using Maxwell’s thermodynamic relations, the isotropic Mie-Grüneisen EOS can be generalized for anisotropic media as follows:
\[
\Gamma_{ij} = \alpha_{ij} \Gamma, \quad \Gamma = \nu \left( \frac{\partial p}{\partial \varepsilon} \right)_T\varepsilon_{ij},
\]

(19)

where the pressure \(p\) is defined by the constitutive equations (10) and \(\varepsilon = \frac{1}{3} \varepsilon_v\) is the isotropic strain.

**An anisotropic EOS**

The equations (10) define the correct generalized "pressure" for the elastic regime. To provide an appropriate description for general anisotropic materials behavior at high pressures, the pressure \(p\) related to the volumetric deformations is described by \(p^{EOS}\) (18, 20). Therefore, an appropriate description of generalized hydrostatic "pressure" at high pressures has the following form:
\[
p^* = p^{EOS} + \frac{\beta_{ij} \tilde{S}_{ij}}{\delta_{kl} \alpha_{kl}}, \quad \sigma_{ij} = -p^* \alpha_{ij} + \tilde{S}_{ij},
\]

(21)

which also describes correctly the medium’s behavior at small volumetric strains. To be consistent with the definition of the isotropic bulk speed of sound, the following definitions of the first \(c_I\) and the second \(c_{II}\) bulk speed of sound for anisotropic medium are assumed:
\[
c_I = \sqrt{\frac{K_C}{\rho_0}}, \quad c_{II} = \sqrt{\frac{K_S}{\rho_0}},
\]

(22)

where the generalized bulk moduli \(K_C, K_S\) are defined according to (13) and (15) respectively. Parameters \(c \in \{c_I, c_{II}\}, S_1, S_2, S_3, \gamma_0, a\) represent material properties which define its EOS (1). A description of their numerical values for AA7010-T6 is shown in Table I.
A NON-ASSOCIATED ANISOTROPIC PLASTICITY MODEL

The main aspects of a phenomenological strength model can be characterized by a yield criterion representing a surface that separates the elastic and plastic regions of the stress space, a flow potential gradient that represents the direction of plastic strain rate, a strain hardening rule and that plastic flow is incompressible.

An anisotropic yield surface

Following the research of Spitzig and Richmond [31], and Stoughton and Yoon [32], the mathematically consistent yield function of a fully anisotropic material based on generalized decomposition of the stress tensor is developed:

\[
F(\bar{\sigma}_{ij}) = \Psi(\bar{\sigma}_{ij}) (1 + \chi p^*) \leq Y(\bar{\varepsilon}_p),
\]

(23)

where \( \Psi(\bar{\sigma}_{ij}) \) is described by generalized Hill’s yield functions:

\[
\Psi^2(\bar{\sigma}_{ij}) = F \left( \alpha_3 \bar{\sigma}_2 - \alpha_2 \bar{\sigma}_3 \right)^2 + G \left( \alpha_1 \bar{\sigma}_3 - \alpha_3 \bar{\sigma}_1 \right)^2 + H \left( \alpha_{22} \bar{\sigma}_{11} - \alpha_{11} \bar{\sigma}_{22} \right)^2 + 2N \bar{\sigma}_{12}^2 + 2L \bar{\sigma}_{23}^2 + 2M \bar{\sigma}_{13}^2,
\]

(24)

where \( \bar{\sigma}_{ij} \) is the generalized deviatoric stress tensor (\( \bar{\sigma}_i = \bar{\sigma}_{ii}, i = 1, 2, 3 \)); \( \alpha_{ij} \) is the generalized Kronecker’s symbol \( \delta_{ij} \) (\( \alpha_i = \alpha_{ii}, i = 1, 2, 3 \)). The material constants \( \chi, F, G, H, N, L, M \) are specified in terms of selected initial yield stresses in uniaxial tension, compression, and equibiaxial tension. It is important to note that plasticity model [24] is naturally independent from the generalized hydrostatic pressure and therefore, the following equality can be written:

\[
\Psi(\bar{\sigma}_{ij}) \equiv \Psi(\sigma_{ij}), \quad \sigma_{ij} = \sigma^* \alpha_{ij} + \bar{\sigma}_{ij}, \quad \sigma^* \neq 0,
\]

(25)

where \( \sigma_{ij} \) is the stress tensor. In this paper, a uniaxial strain state (one-dimensional reduced mathematical formulation in strain space) and the adiabatic approximation assumptions are considered for modelling shock waves propagation in anisotropic solids. Therefore, material parameters and their numerical values for AA7010-T6 are taken as presented in Table I.

An anisotropic plastic potential

A flow potential gradient that represents the direction of plastic strain rate is described by the classical Hill’s anisotropic plastic potential:

\[
\Pi(\sigma_{ij}, \gamma_{ij}) = \left[ F (\sigma_{22} - \sigma_{33})^2 + G (\sigma_{33} - \sigma_{11})^2 + H (\sigma_{11} - \sigma_{22})^2 + 2N \sigma_{12}^2 + 2L \sigma_{23}^2 + 2M \sigma_{13}^2 \right]^{1/2} - \sigma_{ii},
\]

(26)

and has a strain-rate dependent constant \( \sigma_{ii} \) including hardening modulus for plastic potential; \( \gamma_{ij} \) is the back stress for plastic potential, \( D^p_{ij} \) is the plastic strain rate tensor. It is assumed that the parameters \( F, G, H, N, L, M \) can be determined from the anisotropy parameters \( R, P, Q_{23}, Q_{31} \) and \( Q_{12} \) as for the Hill’s yield function [33]. The constitutive equations are integrated using the tangent stiffness matrix. The numerical values for plastic potential parameters were taken from [34].

SIMULATION OF ANISOTROPIC SHOCK WAVE PROPAGATION

The plane shock-wave technique provides a powerful tool for studying material properties at different strain rates [14, 11, 21, 20]. The characteristics as spall pressure, shock velocity, particle velocity, Hugoniot elastic limit, thickness of the spall section, time to spall, and free surface velocity of the spall section can be measured.
Description of Experiment

The flyer plates were launched using a 75 mm bore, 1 m long and 50 mm bore, and 1 m long single stage gas gun the Royal Military College of Science [15]. The shock propagation in the target is monitored using manganin stress gauges, placed between target plate and PMMA (poly methylmethacrylate) plate within the target assembly. The results from the stress gauges were converted by N. Bourne and J. Millett to in material (Target) values $\sigma_M$, using the shock impedances of the target $A_T$ and PMMA $A_P$, via the well-known relation

$$\sigma_M = \frac{A_T + A_P}{2A_P} \sigma_P,$$

(27)

where $\sigma_P$ is the stress gauges values. The 2.5mm thick flyer plates of 6082-T6 (dural) were impacted onto the targets (test material AA 7010-T6) over the velocity range 234 to 895, inducing stresses in the range 2.7 to 7.2 GPa. The aluminium alloy 6082-T6 was chosen as the flyer due to the close similarity in density and wave speeds, so that the impact experiments were near symmetrical [34]. The elastic material properties of 7010-T6 can be found in [34]. Material properties of plates 6082-T6 and PMMA can be found in [19].

Using a finite-difference wave propagation code [35], numerical simulations of plate-impact test were performed with a 5 mm thick target plate, 2.5 mm thick flyer plate and 5 mm PMMA plate. Based on the characteristics of this plate impact problem, the plates (numerical domains), which are used in the numerical simulation, are modelled as 1D bars [35]. The mesh resolutions were sufficient to allow the resolution of all the relevant elastic and plastic waves in the target and flyer. The stress time histories were recorded in the middle of the target plate and at the back of the test specimen (the first FD element in the PMMA connected to test plate).

Shock wave propagation in 7010 T6 anisotropic aluminium alloy

The experimental data for AA7010 T6 presented here correspond to the plate impact test performed by N. Bourne and J. Millett at Royal Military College of Science (published in [34]) with impact velocities of 450 m/s and 895 m/s. Figures 1 and 2 show the comparison between experimental data and the numerical simulation resulting from the new anisotropic equation of state and non-associated anisotropic plasticity model for the longitudinal and transverse cases.

The experimental values, 0.39 GPa and 0.33 GPa for elastic response from the longitudinal and short transverse directions, respectively figures 1 and 2 are in good correlation with the modelled values of the HEL longitudinal - 0.395 GPa and short transverse - 0.333 GPa. The errors with respect to the experimental values are 1.4 % and 0.9 %, respectively to the longitudinal and short transverse directions. Further comparison shows that the stress pulse width (approximately, 0.81 µs ) and release trace are in good agreement with the experiment as well (see fig. 1 and 2). Besides, another important characteristic, the arrival time to the HEL and the plastic wave velocity are in good correlation with experimental data. The main conclusion obtained from these results
is that the non-associated anisotropic plasticity model, as it stands, is suitable for simulating elastoplastic shock wave propagation in anisotropic solids. Different HELs are obtained when the material is impacted in different directions; their excellent agreement with the experiment demonstrates adequateness of the proposed anisotropic plasticity model. However, further work is required both in the experimental and constitutive modelling areas to find a better description of anisotropic material behavior and, particularly, Hugoniot stress level.

CONCLUSIONS

The EOS proposed in this paper represents a physical generalization of the classical Mie-Grüneisen equation of state for isotropic materials. Based on the $\alpha - \beta$ generalized decomposition of stress tensor, the modified Mie-Grüneisen equation of state combined with non-associated plasticity model forms a system of constitutive equations suitable for shock wave propagation in single crystals and polycrystalline alloys. The behavior of the aluminum alloy 7010-T6 under shock loading conditions was investigated. A comparison of the experimental HELs with numerical simulation shows an excellent agreement (maximum error is 1.4%). Furthermore, the good agreement of the general pulse shape and Hugoniot stress level suggests that the EOS is performing satisfactorily. The significance of the proposed strength model includes also the distortion of the yield function shape in tension, compression and in different principal directions of anisotropy (e.g., $0^\circ, 90^\circ$) which can be used to describe the anisotropic strength differential effect (anisotropic SDE). However, further development of the constitutive equations taking into account strain rate sensitivity is required.

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