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EQUATION OF STATE OF ALUMINUM-IRON OXIDE (Fe_2O_3) – EPOXY COMPOSITE: MODELING AND EXPERIMENT

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EQUATION OF STATE OF ALUMINUM – IRON OXIDE (Fe₂O₃) – EPOXY COMPOSITE: MODELING AND EXPERIMENT

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Abstract. We report on the investigation of the equation of state of an 2Al+Fe₂O₃+ 50 wt.% epoxy composite in the 2-23 GPa pressure range. An explosive loading technique, with piezoelectric pins to measure the shock velocity in the sample and in a donor material, was used for experiments exceeding 5 GPa. Gas gun experiments were performed on the same composites at lower pressures, using PVDF stress gauges to record the input and propagated stresses and the shock velocity based on the time of travel through the sample thickness. The experimental results are compared to numerical simulations of shock compression in discrete particle models. Model results are in agreement with experimental results.

Keywords: Equation of state, aluminum-iron oxide, epoxy, finite element modeling, shock waves.

PACS: 62.50.+p, 64.30.+t, 81.05.Qk

INTRODUCTION

Equation of state (EOS) studies on epoxy-based particulate (metal, oxide, or their mixtures) composite systems used for structural applications have been reported because of their low density and relatively high strength [1-3]. Shock compression of 2Al+Fe₂O₃ powders [4] (traditional thermite system) has shown a response dominated by the dissimilar compressibilities of the respective metal and oxide constituents, but no obvious evidence of reaction at pressures less than 15 GPa. In this paper, EOS measurements are performed on 2Al+Fe₂O₃+50 wt.% epoxy composites using gas gun and explosive loading configurations. Numerical models are constructed to simulate shock wave propagation in discrete particle

mixtures, and establish Hugoniot relations, which are compared to those measured in experiments.

EXPERIMENTAL PROCEDURE

EOS experiments were conducted on 2Al+Fe₂O₃+50wt.% epoxy composites utilizing planar impact experiments using the Georgia Tech gas gun facility and plane wave lenses with explosive loading at AFRL, Eglin AFB, FL. The samples were composed of 2 μm spherical aluminum particles and agglomerates of 0.3 μm blocky iron oxide, which were mixed with Shell Epon 826 Resin/DEA hardener and cast-cured. Castings in the form of 50 mm diameter rods were prepared from which 2 mm thick disks were sectioned and used for the EOS experiments.

Four experiments, listed in Table 1, were conducted using the 80 mm diameter single-stage

light-gas gun with impact velocities between 500 and 950 m/s [5]. PVDF gauges mounted on the front and rear surfaces of the sample provided an input and propagated stress profile. The travel time between the two gauges was used to determine the shock wave speed in the sample. Assuming hydrodynamic conditions and steady state wave propagation through the sample, the measured input stress and the shock wave speed, combined with the jump conditions, were used to determine the U_s-U_p , and $P-U_p$ states. Ten EOS experiments, detailed in Table 1, were conducted using explosive plane wave lenses (PWL) in conjunction with TNT, Octol, or Baratol pads for loading at higher shock pressures. A donor material, and optionally a PMMA attenuator, is placed on the explosive pad. The sample is then placed in contact with the donor. In these experiments, the shock velocity in the donor and the sample is measured using piezoelectric pins, which are placed in flat-bottomed holes drilled at differing depths. In experiments JJH24-JJH26, three sets of three piezoelectric pins were used in both the sample and the donor, and two sets of three pins each were used in the other experiments. Using the shock velocity in the donor and the sample, the remaining Hugoniot properties for the sample were determined using impedance matching.

MODELING AND SIMULATION

Shock compression of discrete particle systems has been studied extensively by Benson et al. [6-9] using numerical techniques. In this study, shock wave propagation through simulated microstructures of $2Al+Fe_2O_3+epoxy$ composites was used to calculate $P-U_p$ and U_s-U_p relations using finite element (FE) simulation. Hugoniot relations are calculated in the simulations. A detailed description of the methods utilized in these simulations is described elsewhere [10].

The microstructures were reconstructed by, first, generating discrete sets of ‘particles’ (Al particles, Fe_2O_3 agglomerates, and voids) with diameters conforming to lognormal size distributions matching those quantitatively obtained from actual microstructures. The number of particles generated for each phase was controlled by the prescribed volume fractions of

the statistical volume element (SVE). Next, particles were sequentially added to the domain using a constrained Poisson process. A simulated annealing technique [11] was used to evolve nearest-neighbor distributions in the aluminum phase to those estimated from experimental microscopy. Volumes of the SVE not occupied by the particles or inclusions were filled with epoxy. The components of a sample realization of the model SVE are shown in Figure 1; the dimensions of the SVE ($22\ \mu m \times 11\ \mu m$) were selected based on a sensitivity analysis.

The FE simulations were performed using the 2-D multi-material Eulerian hydrocode, Raven [12]. Arbitrary Lagrangian-Eulerian (ALE) formulations were used so that the severe element distortions encountered in traditional Lagrangian formulations are avoided. The shock compression of the composite was idealized by the passage of a single, ostensibly 1-D shock wave. Here, the plane strain assumption was invoked to reduce the true 3-D nature of shock loading to a computationally tractable 2-D case (particles in the 2-D cross section are considered as cylinders in 3D, i.e., extended into the plane). The initial boundary value problem, which aims to replicate idealized shock loading, is depicted in Figure 1. A compressive shock wave is generated by applying a velocity boundary condition to the left surface of the SVE. Symmetry planes serve as the boundary conditions for the top and bottom surfaces of the model. A fixed boundary condition is imposed on the right surface.

The stress-strain response of each phase was decomposed into hydrostatic and deviatoric

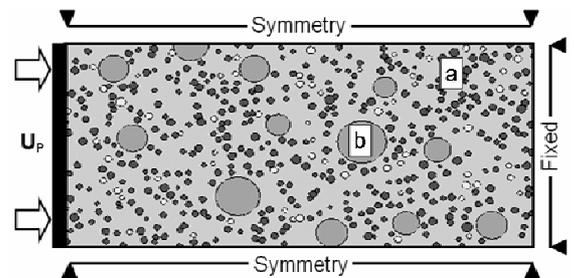


FIGURE 1. An SVE of the $2Al+Fe_2O_3+epoxy$ composite is depicted with boundary conditions applied for 1-D shock wave propagation. Markers indicate: (a) Fe_2O_3 agglomerates and (b) Al particles; white circular entities are pores.

components. The Mie-Grüneisen EOS is used to model the hydrostatic response of the Al and epoxy phases; the Murnaghan EOS [13] was used to model the hydrostatic response of the iron oxide phase. A constitutive model for high-purity FCC metals (based on thermally-activated mechanisms) [14] was used to model the deviatoric stress-strain response of the aluminum phase. The Hasan-Boyce model [15] was used as the strength model for the epoxy phase. A phenomenological constitutive model for iron oxide is not available in the open literature. Therefore, a simple elastic-plastic strength model, consisting of an initial linear elastic response followed by linear isotropic strain-hardening, was adopted.

RESULTS AND DISCUSSION

The experimental results are presented in Table 1 and plotted in the form of $U_s - U_p$ and $P - U_p$ relations in Figure 2. The shock velocity values correspond to those measured based on the time of travel between the input and propagated stress gauges in the gas gun experiments and between piezoelectric pins in explosive loading experiments. In Figure 2 (a), the line fitted to the data points reveals a smooth trend without any obvious discontinuities. However, there is considerable scatter in the data at higher pressures, which may be due to the inherent differences in different samples of the same composite material. A linear fit to the $U_s - U_p$ plot results in a C_0 , the dynamic bulk sound speed, of 3.27 km/s and S , an empirical parameter, of 1.04 for the 2Al+Fe₂O₃+epoxy composite. The fit depicted in Figure 2 (b) is the translation of the linear relationship determined from $U_s - U_p$ data to the $P - U_p$ space. This assumes the stress measured by the PVDF gages is equivalent to the hydrodynamic pressure response, which was shown to be true for alumina – epoxy composites [3].

The smooth trends exhibited by the data from both sets of experiments (i.e., no discontinuities in the Hugoniot) indicate that there are no chemical or physical changes occurring in the 2Al+Fe₂O₃+epoxy composite samples at pressures up to 23 GPa. Absence of a chemical reaction, in an otherwise highly reactive system, may be expected due to the presence of a large volume

fraction of epoxy, which may inhibit intimate mixing and contacts between the aluminum and iron oxide powders.

A set of simulations was performed with particle velocities matched to those achieved in the experiments. Results were averaged for three realizations of the microstructure at each prescribed particle velocity. The $U_s - U_p$ and $P - U_p$ relations for the 2Al+Fe₂O₃+epoxy composite, shown in Figure 2 (a) and (b), were calculated by tracking the position of the shock front with respect to time. Here, an averaging scheme was used to define the location of the shock front, as shock waves do not remain precisely planar when propagating through heterogeneous media. The stationary pressure was calculated by averaging the pressures of all elements behind the shock-wave front. As shown in Figure 2 (a), shock velocity calculations agree with experimental data in the high-velocity regime, $U_p > 1.500$ km/s, with differences less than 8%; the low-velocity regime, $0.364 \text{ km/s} \leq U_p \leq 0.607$ km/s, contains larger differences, up to 14%. Pressure calculations (Figure 2(b)) show excellent agreement with experiments in the low-velocity regime, with differences less than 7%; in the high-velocity regime, differences are larger, up to 12%.

CONCLUSIONS

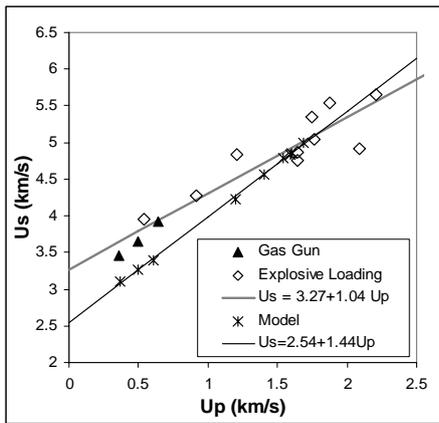
EOS experiments on cast 2Al+Fe₂O₃+50wt.% epoxy cast composite samples were performed at pressures up to ~23 GPa. The reactive particle systems do not exhibit any signs of shock-induced chemical reactions or physical changes in this pressure regime. Numerical models of the shock compression of discrete particle mixtures show reasonable correlation with experimental data; differences between Hugoniot calculations and measurements are less than 15% for the $U_s - U_p$ and $P - U_p$ relations.

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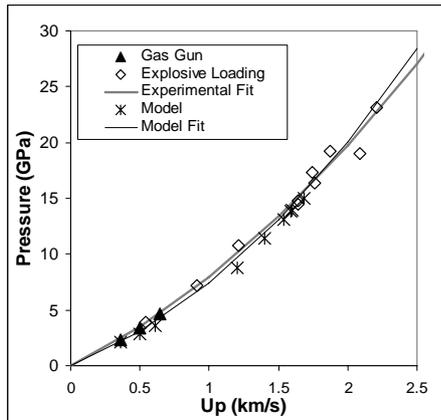
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TABLE 1. Equation of state test results on $2\text{Al}+\text{Fe}_2\text{O}_3+\text{epoxy}$ composites (ρ_0 is the initial density, U_s is the shock velocity, U_p is the particle velocity, and P is the pressure). The shaded columns are experimentally measured parameters. Measurement uncertainties are due to assembly tolerances, sample variations, and measurement limitations.

Exp. No.	Test Configuration	Impactor	Driver	Vp (m/s)	ρ_0 (g/cc)	U_s (km/s)	U_p (km/s)	P (GPa)
0308	Gas Gun	Cu	Cu	553 ± 43	1.865	3.465 ± 0.009	0.364 ± 0.004	2.35 ± 0.35
0311	Gas Gun	Cu	Cu	714 ± 89	1.850	3.653 ± 0.008	0.499 ± 0.004	3.37 ± 0.12
0403	Gas Gun	Cu	Cu	944 ± 4	1.859	3.917 ± 0.010	0.607 ± 0.005	4.66 ± 0.31
JJH8	PWL/TNT		Al		1.850	5.036 ± 0.081	1.760 ± 0.127	16.40 ± 1.24
JJH9	PWL/TNT/PMMA		Al		1.850	4.841 ± 0.524	1.209 ± 0.173	10.82 ± 1.95
JJH10	PWL/TNT		PMMA		1.850	4.750 ± 0.150	1.644 ± 0.328	14.45 ± 2.92
JJH11	PWL/Octol		Al		1.850	5.353 ± 0.368	1.746 ± 0.033	17.29 ± 1.26
JJH12	PWL/Octol/PMMA		Al		1.850	4.921 ± 0.589	2.087 ± 0.469	19.00 ± 4.85
JJH13	PWL/Octol		PMMA		1.850	5.655 ± 0.564	2.207 ± 0.304	23.09 ± 3.03
JJP22/23	PWL/TNT		Al		1.850	5.541 ± 0.069	1.874 ± 0.212	19.21 ± 2.20
JJH24	PWL/TNT		Cu		1.850	4.278 ± 0.051	0.913 ± 0.318	7.22 ± 2.52
JJH25	PWL/Baratol		Cu		1.850	3.955 ± 0.195	0.538 ± 0.151	3.94 ± 1.12
JJH26	PWL/Octol		Cu		1.850	4.862 ± 0.069	1.642 ± 0.162	14.77 ± 1.48



(a)



(b)

FIGURE 2. (a) Shock velocity–particle velocity (U_s-U_p) and (b) pressure–particle velocity ($P-U_p$) relation for $2\text{Al}+\text{Fe}_2\text{O}_3+\text{epoxy}$ composite from experiment and numerical model.

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