AFRL-RW-EG-TP-2012-009

Mesoscale Simulations of Particle Reinforced Epoxy-Based Composites

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25 July 2012

Interim Report

AIR FORCE RESEARCH LABORATORY, MUNITIONS DIRECTORATE

Air Force Materiel Command ■ United States Air Force ■ Eglin Air Force Base

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REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1. REPORT DATE *(DD-MM-YYYY)*
25 July 2012

2. REPORT TYPE
Interim

3. DATES COVERED *(From - To)*
July 2009 – July 2011

4. TITLE AND SUBTITLE
Mesoscale Simulations of Particle Reinforced Epoxy-Based Composites

5a. CONTRACT NUMBER

5b. GRANT NUMBER

5c. PROGRAM ELEMENT NUMBER
62102F

6. AUTHOR(S)
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5d. PROJECT NUMBER
4347

5e. TASK NUMBER
95

5f. WORK UNIT NUMBER
05

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
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[4]School of Materials Science and Engineering, Georgia Tech, 771 Ferst Drive NW, Atlanta, GA 30332

8. PERFORMING ORGANIZATION REPORT NUMBER
AFRL-RW-EG-TP-2012-009

9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES)
Air Force Research Laboratory, Munitions Directorate
Ordnance Division
Energetic Materials Branch (AFRL/RWME)
Eglin AFB FL 32542-5910
Technical Advisor: Dr. Jennifer L. Jordan

10. SPONSOR/MONITOR'S ACRONYM(S)
AFRL-RW-EG

11. SPONSOR/MONITOR'S REPORT NUMBER(S)
AFRL-RW-EG-TP-2012-009

12. DISTRIBUTION / AVAILABILITY STATEMENT
Distribution A: Approved for public release; distribution unlimited. Approval Confirmation 96 ABW/PA # 96ABW-2011-0363, Dated, August 2, 2011

13. SUPPLEMENTARY NOTES
DISTRIBUTION STATEMENT INDICATING AUTHORIZED ACCESS IS ON THE COVER PAGE AND BLOCK 12 OF THIS FORM.

14. ABSTRACT
Polymer matrix composites reinforced with metal powders have complex microstructures that vary greatly from differences in particle size, morphology, loading fractions, etc. The effects of the underlying microstructure on the mechanical and wave propagation behavior of these composites during dynamic loading conditions are not well understood. To better understand these effects, epoxy (Epon826/DEA) reinforced with different particle sizes of Al and loading fractions of Al and Ni were prepared by casting. Microstructures from the composites were then used in 2D plane strain mesoscale simulations. The effect of varying velocity loading conditions on the wave velocity was then examined to determine the Us-Up and particle deformation response as a function of composite configuration.

15. SUBJECT TERMS
Split Hopkinson pressure bar, pressure dependence, high strain rate, poly(vinyl chloride)

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
a. REPORT	b. ABSTRACT	c. THIS PAGE			Jennifer L. Jordan
UNCLASSIFIED	UNCLASSIFIED	UNCLASSIFIED	UL	11	19b. TELEPHONE NUMBER *(include area code)* 850-882-8992

Standard Form 298 (Rev. 8-98)
Prescribed by ANSI Std. Z39.18

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MESOSCALE SIMULATIONS OF PARTICLE REINFORCED EPOXY-BASED COMPOSITES

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Abstract. Polymer matrix composites reinforced with metal powders have complex microstructures that vary greatly from differences in particle size, morphology, loading fractions, etc. The effects of the underlying microstructure on the mechanical and wave propagation behavior of these composites during dynamic loading conditions are not well understood. To better understand these effects, epoxy (Epon826/DEA) reinforced with different particle sizes of Al and loading fractions of Al and Ni were prepared by casting. Microstructures from the composites were then used in 2D plane strain mesoscale simulations. The effect of varying velocity loading conditions on the wave velocity was then examined to determine the Us-Up and particle deformation response as a function of composite configuration.
Keywords: Particulate Composites, Shock, Mesoscale Simulations
PACS: 62.50.Ef, 81.05.Qk, 81.70.Bt

INTRODUCTION

Particle reinforced polymer composites such as Al/Fe_2O_3/Epoxy [1] and Al/W/PTFE [2] are increasingly being studied for use as structural energetic materials designed to combine mechanical strength with reactive property characteristics from multiple materials into a single system designed to be inert under static loads and react and release energy under dynamic impact conditions [2, 3].

Factors such as particle size, morphology, and volume fraction are known to affect the mechanical behavior of particle reinforced composites. In a study conducted on nano-Al particle reinforced polymer composites [4], reactions were observed to occur at impact velocities < 150 m/s and were dependent on the volume fraction of the nano-Al. In computational studies on Ni/Al particulate composites [5] the effects of particle morphology on reaction mechanisms were investigated. They found mixtures containing Ni-flake particles vs. spherical had significant flattening of the Al particles and opened up more surface area to come into contact with the Ni. One major difference between these granular composites and more homogeneous polymer matrix composites is that voids are largely not present. As such the mechanisms of mechanical mixing that lead to reactions under shock wave propagation for polymer-based composites are potentially different and need to be investigated.

In this work the interaction effects of particle size and loading fractions of Ni and Al on the dynamic mechanical behavior of epoxy cast particulate composites under shock loading conditions are examined. Computational efforts are specifically used to examine the shock wave propagation at the mesoscale to better understand the deformation of the composite constituents.

Shock Compression of Condensed Matter - 2011
AIP Conf. Proc. 1426, 175-178 (2012); doi: 10.1063/1.3686248

TABLE 1. Composite configurations used to obtain and import 2D microstructures in ALE3D.

Material	Al Particle Size (μm)	Al Vol. Frac. (%)	Ni Vol. Frac. (%)
EAN-1	52	40	10
EAN-2	5	40	10
EAN-3	5	20	10
EA-1	52	40	0
EA-2	52	20	0

MICROSTRUCTURE GENERATION

Due to their well known properties, Ni and Al were chosen as reinforcing particles in an epoxy matrix. The average Al particle size was varied between 5 and 52μm, the volume fraction of Al between 0.20 and 0.40, and the volume fraction of Ni (47μm) from 0.00 to 0.10 (see Tab. 1). Representative microstructure images from samples were converted into shape files used in 2D plane-strain simulations in ALE3D. While simulations implementing the 'real' microstructures would be ideal, in order to have a greater control over the mesh resolution a MATLAB script converted the real microstructure into an idealized one with each particle defined as a sphere. This retained the volume fraction to within 1% of the original microstructure and kept the same spatial distribution of the particles. Two idealized microstructures are shown in Fig. 1 for materials EAN-1 and EAN-2 and an overlay of an idealized microstructure on top the original microstructure in Fig. 2 for composite EA-2. A mesh resolution study determined an element size of 2.0 and 0.5μm in each direction was sufficient to capture an accurate response for composites containing the large and small Al particles respectively.

SIMULATION SETUP

The microstructure simulation domain was chosen to contain at least the homogeneous length scale of the microstructure in each direction and have an aspect ratio of 2:1 (w:h). This amounted to 1000 and 250μm in the horizontal direction for composites containing larger and smaller Al particles respectively. Along the top and bottom sides of the domain a symmetry plane was placed and along the right-hand side a

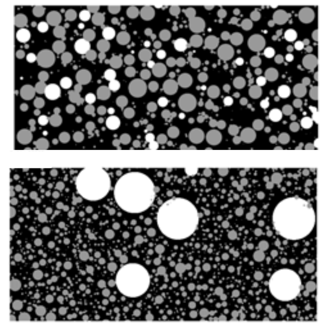

FIGURE 1. Idealized microstructures for EAN-1 (top) and EAN-2 (bot). Ni shown as white particles, and Al gray.

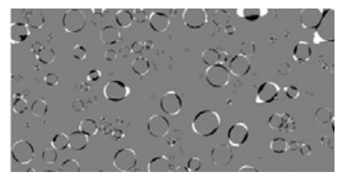

FIGURE 2. Overlay of an idealized microstructure on top of the original microstructure. The black and white regions highlight differences in particle shapes.

free surface boundary condition. To create a shock wave, a Cu driver impacted the domain at velocities between 400 and 1200 m/s to produce different shock *(Us)* and particle *(Up)* speeds. Tracer points were placed along the vertical direction at horizontal distances of .25, .50, and .75 times the domain width to track pressure and stress. See Fig. 3 for a schematic of the boundary conditions.

For Al and Ni the equation of state and strength models implemented were the Mie-Gruneisen and Steinberg-Guinan models respectively with material default parameters set for both Al and Ni. For epoxy a Mie-Gruneisen EOS was used with γ_0 = .763, C_0= 2367 m/s, and S = 1.55. The constitutive behavior of epoxy was defined using a tabular rate hardening model where the flow stress is a function of the equivalent plastic strain $\bar{\varepsilon}_p$ and a power law strain rate dependence through the following equation:

$$Y\left(\bar{\varepsilon}_p, \dot{\bar{\varepsilon}}_p\right) = Y\left(\bar{\varepsilon}_p\right)\left[a + b\dot{\bar{\varepsilon}}_p\right]^m \qquad (1)$$

Here, $\dot{\bar{\varepsilon}}_p$ is the equivalent plastic strain rate, a and b hardening model material constants and m the power law strain rate parameter. Using data from [6]

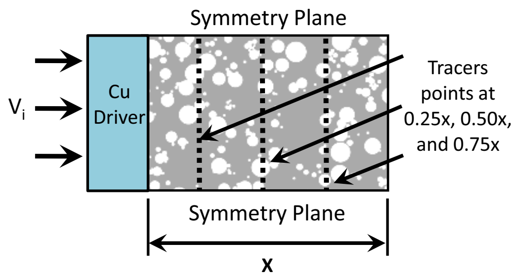

FIGURE 3. Schematic of the boundary and loading conditions used for the 2D plane strain simulations.

this model was applied to the stress-strain curves from strain rates of 134 to 1.4x10^4 s^-1. By using a strain rate of 3.9x10^3 s^-1 as a reference curve a set of values for the parameters were found by minimizing the difference in the peak stress between the experiments and model curves. The values for a, b, and m were determined to be 0.085, 249.0, and 0.14 respectively.

EQUILIBRATION OF PRESSURE

From tracer data the pressure was monitored for the entire duration of the shock wave propagation. In comparing the average shock pressures between EAN-1 with EAN-2 there was little difference in the pressures achieved for each impact velocity (see Fig. 4). However, the variations in pressure were greater for composite EAN-1. This is contrary to what was expected since the Ni and Al particles are closer in size for this material and the pressures are averaged over a much larger vertical distance, 500μm as opposed to 125μm for composite EAN-2. This may be due to more homogeneous distribution of the Al particles when smaller particles are used while holding the volume fraction constant. When comparing the pressure differences between EA-1 and EA-2 there was a decrease in the pressure as the volume fraction of Al decreased.The pressure was 18% larger for the composite EA-1. This was expected since pressure is related to density and there was a marked drop in density as the volume fraction of Al decreased.

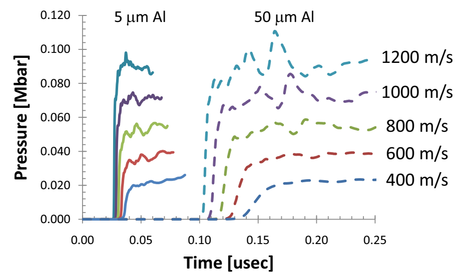

FIGURE 4. Pressure traces for EAN-2 (left) and EAN-1 (right) at the positions 125 and 500μm respectively.

TABLE 2. Us-Up Hugoniot parameters.

Material	S	C_0 [m/s]	Exp. C_0 [m/s]
EAN-1	1.590	2749	2374
EAN-2	1.385	2916	2357
EAN-3	1.708	2990	2079
EA-1	1.478	2968	2475
EA-2	1.417	2822	2280

US-UP RELATIONSHIPS

By determining the time at which the pressure was 0.20x the steady state pressure an average shock velocity was calculated from the distances between tracers. The results of the shock speed calculations were plotted for each composite and velocity with a linear line fit to the data. From these fits, values for S and C_0 were determined using Eqn. 2 that relates U_S with U_P, and the bulk sound speed C_0.

$$U_S = SU_P + C_0 \tag{2}$$

The values for S and C_0 are tabulated in Tab. 2 along with C_0 experimentally determined from ultrasonic sound speed measurements. Despite shifts towards higher shock velocities as the volume fraction of particles increased the composite shock velocities, other than EAN-3, had shock velocities that fell within a 200m/s range with only slight differences in the slopes and no clear influence of particle size or the presence of Ni on the U_S-U_P relationships. This may indicate the contiguous epoxy matrix phase has a dominant role on the shock propagation.

C_0 determined from ultrasonic methods are noticeably lower. This is attributed to the assumption of perfect bonding between the constituents since no interfaces or bond strengths were defined in the simulations. The simulations also have no defects such as microcracks or pores present that would affect the bulk sound speed of the composite.

PARTICLE DEFORMATION

To better understand the mechanisms involved with the mixing of constituents that can lead to a reaction the stresses and strains were monitored as the shock wave propagated through the microstructure domains. For composite EA-1 the stresses of the epoxy and Al particles were found to equilibrate quickly within each phase behind the shock front with no large variations. In all cases the epoxy carried more load than Al and in cases where the composites contained Ni most of the load was carried by Ni. This was an indication that the epoxy can be used to impart more strain into softer phases such as Al.

In the following plots the strains are shown for EA-1 and EAN-2 (see Fig. 5) at the completion of the simulations in which the shock front reaches the free surface for an impact velocity of 800 m/s. For the materials without Ni, the regions with the most plastic strains were located at the Al/epoxy interfaces. The Al appeared to have slight elongation perpendicular to the shock wave propagation direction (towards the right).

For composites containing Ni particles the deformation behavior of Al was drastically different. In regions surrounding Ni extreme strain values (> 400%) were observed at the Ni/Epoxy or Ni/Al interfaces. Al deformed to much larger extents than in composites without Ni and deformed to match the contours of the Ni particles which strained very little. Ni in these types of composites act as rigid anvils that enable much larger strains to be produced in the other less stiff phases. Additionally enhanced 'fluid-like' flow of epoxy and Al was observed to occur between and around the Ni particles. This behavior may act as a primary source of mixing that leads to reactions in epoxy-based composites. More enhanced flow and deformation of Al also occurred in composites with smaller Al particles. This may be due a finite strain field radius produced by the Ni particles. In Fig. 5 the large strains in Al are within approximately one Ni particle diameters. In composites with the larger Al the strain fields are on average only extend up to a radius equivalent to one Al particle diameter.

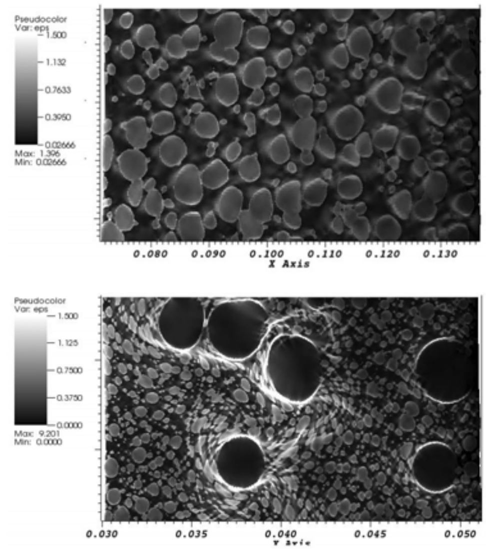

FIGURE 5. Plastic strain plots for EA-1 (top) and EAN-2 (bottom) for an impact velocity of 800 m/s.

ACKNOWLEDGMENTS

Funding was provided by the U.S. Air Force Research Labs, Eglin AFB under contract F08630-03-C-0001.

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