Use of Richtmyer-Meshkov Instability to Infer Yield Stress at High-Energy-Density

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We use the Richtmyer-Meshkov instability (RMI) at a metal/gas interface to infer the metal's yield stress (Y) under shock loading and release. We first model how Y stabilizes the RMI using hydrodynamics simulations with a perfectly-plastic constitutive relation for copper (Cu). The model is then tested with molecular dynamics (MD) of crystalline Cu by comparing the inferred Y from RMI simulations with direct stress-strain calculations, both with MD at the same conditions. Finally, new RMI experiments with solid Cu validate our simulation-based model and infer Y ~0.47 GPa for a 36 GPa shock.

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In the Richtmyer-Meshkov instability (RMI), a shock amplifies perturbations at material interfaces at a rate that depends on the material properties. In melted materials, the RMI is fluid-like and grows linearly in time until nonlinearities reduce the growth rate in an asymmetric manner [1 and references therein]. In materials with strength (i.e. yield stress Y ≠ 0), the RMI growth is arrested and stabilized at an amplitude $h^{max} \propto 1/Y$. Piriz et al [2] (P08) used two-dimensional (2D) simulations of perturbations at a vacuum/metal interface (Atwood number A = +1) to obtain a relation between h^{max}, Y and RMI dynamical parameters. Piriz et al [3] then suggested using the relation to infer an effective Y at high-energy-density, but it has not been tested experimentally nor with real materials. We are studying the complementary metal/gas system (A ~ -1) in which shocks produce ejecta [4-6] in order to develop an RMI-based model for the amount and velocity of ejecta both below and above melt conditions.

Here, we begin our model development by studying the RMI in copper (Cu) with Y ≠ 0 in three steps. First, we use full hydrodynamic simulations (HS) of an ideal Cu-gas system to obtain a relation between h^{max}, Y and RMI dynamical quantities. With A ~ -1, we find it necessary to describe the RMI in the nonlinear regime and with asymmetric growth beyond that done in P08. For clarity, the Cu remains solid with an assigned Y using a perfectly-plastic constitutive relation. Second, we test our model self-consistently using molecular dynamics (MD) simulations by comparing direct measurements of Y with those inferred from MD/RMI simulations. Both are done with MD of single crystalline Cu under similar conditions and realistic material properties. Third, we apply our model to new RMI experiments with polycrystalline Cu below melt to infer a Y that compares favorably with the prediction in ref. [7]. These results are important for describing the hydrodynamics and ejecta in shock-driven applications involving metals.

We first study the strength suppression of the RMI using HS of an idealized Cu/gas system with PAGOSA [8]. PAGOSA is an Eulerian finite-difference multimaterial hydrodynamics code with a variety of thermodynamic, material strength and high-explosive (HE) models. In a configuration like Fig. 1 of ref. [1], we launch a shock in the Cu (A) toward a perturbed interface with a perfect gas (B). The Cu has a density ρ_A = 8.9 g/cc and remains a solid with an assigned constant Y. The gas has little influence due to its low density ρ_B = 1.22 mg/cc $<< \rho_A$ (A = $(\rho_B - \rho_A)/(\rho_B + \rho_A)$ ~ -1) and is given a specific heat ratio γ_B = 5/3. The initial shock satisfies the Cu Hugoniot relation W_i = 3.94 km/s + 1.489 u_3, where W_i is the incident shock speed and u_3 is the trailing particle speed. In characterizing the machined surfaces [5], we find that they are mainly 2D single-mode perturbations. Thus, our HS are 2D and use one wavelength λ ≡ 2π/k = 4.3 cm with 86 zones/λ for numerical convergence, where k is the wavenumber. The initial perturbation has an amplitude h_o^- prior to the shock arrival and $h_o^+ = h_o^- \left(1 - U / W_i\right)$ after the shock transit, where U is the acquired interface speed.

PAGOSA simulations with $Y = 0.5$ GPa are exemplified in Fig. 1 in scaled units (defined below) for 4 values of $k\,h_o^-$. For brevity, the images depict only the interfacial regions with Cu in yellow and gas in black. Each case uses a drive pressure of 160 GPa to produce a right-moving shock with $u_3 = 2.5$ km/s, $W_i = 7.64$ km/s and $U = 5.26$ km/s and, on release, a Cu density of 8.3 g/cc and temperature T ~1300 °K. The RMI growth rate increases with $k\,h_o^-$ and is negative for A ~ -1 [9]. Thus, the perturbation inverts phase after the shock compression, and then grows asymmetrically due to A = -1 and at a reduced rate due to Y. To understand this complex evolution, we first clarify our geometry. As shown in the first image, the initial perturbation is taken to be $Z(t = 0^-) = h_o^- \cos(kx)$ relative to a flat interface ($Z \equiv 0$) with $Z > 0$ to the right. The shock first compresses the perturbation to $h_o^+ / h_o^- \sim 0.33$ with the same phase since $U < W_i$. The perturbation then grows negatively so that the depression in the center ($kx = \pi$) becomes a protrusion that we call a spike of heavy material. The initial protrusions at $kx = 0$ and 2π become depressions that we call bubbles of light fluid. Such a slow phase inversion is predicted by linear theory [9] and observed experimentally [10] for A < 0. In our convention, the scaled spike (bubble) amplitude kh_{Sp} (kh_{Bu}) starts negative (positive) and 'grows' in the opposite direction. To distinguish bubbles and spikes, we perform separate simulations with flat interfaces for Z(t). Time is scaled by the peak bubble growth rate $V_{Bu}^o \equiv \max\left(dh_{Bu} / dt\right)$, namely, as $\tau \equiv k|V_{Bu}^o|t$, because we find that V_{Bu}^o agrees with the Meyer-Blewett [11] growth rate $V_{MB} = -U\,k\left(h_o^- + h_o^+\right)/2$ for A = -1 and $k\,h_o^- < 0.5$. Conversely, the harmonics 'accelerate' the spikes in the fluid regime to a velocity

$$V_{Sp}^o \equiv \max\left(dh_{Sp} / dt\right) \Rightarrow V_{Bu}^0 \sqrt{3\left(kh_o^- + 1\right)/\left(3kh_o^- + 1\right)} \quad [12, 13, 1].$$

Figure 1 shows that bubbles and spikes evolve quite differently for A ~ -1 and $Y \neq 0$. The bubbles always saturate but the amplitude increases with $k\,h_o^-$ since it determines the RMI growth rate. The spikes saturate and remain contiguous with the bulk Cu only for $k\,h_o^- \leq 0.18$. For $k\,h_o^- = 0.22$, the spikes detach from the bulk Cu but without further change in morphology. For $k\,h_o^- = 0.4$, they continue to elongate and eventually disintegrate into particles. These results suggest an ejecta transition in which the saturated bubbles (spikes) determine the amount (velocity) of the ejecta, even for unmelted materials.

We generalized the results in Fig. 1 using PAGOSA simulations with different values of W_i, $k\,h_o^-$ and Y. The results are summarized in Fig. 2 by plotting the scaled saturation amplitudes $\left|kh_{Bu}^{max}\right|$ and $\left|kh_{Sp}^{max}\right|$ vs. the RMI strength parameter

$$k\,h_Y \equiv \frac{\rho_A}{Y}\left|V_{Sp}^0\right|^2 \tag{1}$$

The spikes are well described by the least-squares fit (dashed line in Fig. 2)

$$\left|kh_{Sp}^{\max}\right| = 0.08 + 0.24\;kh_Y \tag{2}$$

Our coefficient of 0.24 for A = -1 is smaller than the 0.29 of P08 for A = +1, which is reasonable since RMI growth rates differ with the sign of A. Our intercept of 0.08 may be related to the amplitude ξ_0 defined by P08 where strength becomes important. Since both are small and somewhat ambiguous, we estimate an average RMI (perfectly-plastic) yield from Eq. 2 to be

$$Y_{RM} \sim 0.24\,\rho_A\,\frac{\left|V_{Sp}^0\right|^2}{k\,h_{Sp}^{\max}} \tag{3}$$

for A ~ -1, with an uncertainty of 10-20% for observations near $kh_{Sp}^{\max} \sim 1$. We focus Eqs. 1-3 on spikes because they grow faster and to larger amplitudes than bubbles for $|A| \sim 1$, as seen in ref. [1] and Fig. 1. This makes spikes easier to observe, as shown below. In addition, the spikes saturate at an amplitude that increases simply with kh_Y and they exhibit a dramatic transition to unbounded secular growth when $kh_Y \geq$ 10 ± 1. The uncertainty arises since we observe 3 cases with $kh_Y \sim$ 9.5-11.5 (diamonds) where the spikes saturate and 2 cases at $kh_Y \sim$ 10 (arrows) that grow indefinitely. In contrast, the bubbles saturate at smaller amplitudes and for all kh_Y. Even in the fluid regime ($kh_Y \Rightarrow \infty$), the bubble velocity decays as 1/kt asymptotically. By mass conservation, this asymmetric growth causes the spikes to become very narrow and eventually disintigrate into ejecta particles. This will form the basis for a future ejecta source model.

We now test our RMI strength-suppression model with MD by comparing Y_{RM} from MD/RMI simulations with a direct calculation of Y, both with the SPaSM code [14] at similar T and strain rate (SR). MD can describe small-scale mixing and material damage from void growth in an *ab-initio* manner because they describe atomic interactions. We use an embedded atom method [15] for Cu with a 0.5 nm potential cutoff radius. The domain is 2.6 nm deep to reduce edge effects and 2D in X-Z with λ = 257 nm and 50-60 million atoms in an fcc lattice next to a vacuum (A = -1). Figure 3 shows MD/RMI results for an 83 GPa incident shock with u_3 = 1.5 km/s, W_i = 6 km/s and U = 3 km/s. On release, the Cu at ~8.7 g/cc and T

4

~1003 °K remains below the melt temperature (1350 °K). The initial perturbations at kh_o^- = 1 are first compressed to kh_o^+ ~ 0.5 as expected. They then grow with V_{Bu}^o ~ -0.44 ± 0.08 km/s and V_{Sp}^o ~ 0.6 ± 0.1 km/s. Both are smaller than V_{MB} ~ 2.25 km/s due to nonlinearities [1] and strength. The strength-induced saturation amplitudes $\left|kh_{Bu}^{max}\right|$ ~ kh_{Sp}^{max} ~ 0.67 are similar because kh$_Y$ is small, but the asymmetry increases with kh$_Y$ in our MD/RMI simulations, similar to Figs. 1 and 2. Inserting kh_{Sp}^{max} and V_{Sp}^o into Eq. 3, we obtain Y$_{RM}$ = 1.1 ± 0.3 GPa. We believe the differences between Figs. 1 and 3 occur because kh$_Y$ ~ 2.7 is small compared to 4.6, 11.3, 17.6 and 63.4 for the four cases in Fig. 1, and the yield curve is more realistic.

The stress-strain curve is calculated directly with MD, as shown in Fig. 4 for the conditions in Fig. 3. A Cu crystal (36x289x2 nm) is prepared at T = 1003 °K and the resistance force (stress) is measured while the sample is sheared at an SR ~ ns^{-1} (SR varies from 0 to kV$_{Sp}$ ~ 10 ns^{-1} in our MD/RMI simulations). In Fig. 4, Y varies in the range of 1.2-1.5 GPa for strains < 0.2 and decreases to 0.65 GPa at the peak strain $\left|kh_{Sp}^{max}\right|$ ~ 0.7 in Fig. 3 due to plastic work since T increases by ~200 °K . For strains of 0 to 0.7, we obtain an average Y = 0.95 ± 0.3 GPa which is consistent with Y$_{RM}$ from our MD/RMI simulations. These values are also consistent with the peak Y ~ 1.4 GPa obtained in refs. [7 and 16] for our conditions.

Finally, we apply our model to Cu experiments [6] driven by HE and diagnosed with proton radiography (pRad) and laser Doppler velocimetry (LDV), as shown in Fig. 5. The HE generates a 36 GPa shock in a 6 mm thick Cu plate with W$_i$ ~ 5 km/s and U = 1.46 km/s. U is measured directly with LDV on 3 flat regions (black arrows) while W$_i$ and T ≤ 500 °K are inferred from Cu Hugoniot relations. There are 4 sets of initial perturbations with λ = 0.55 mm and kh_o^- = 0.75, 0.12, 0.35 and 1.5 to span kh$_Y$. The pRad images show the perturbations with kh_o^- ≤ 0.35 being stabilized by Y whereas those with kh_o^- ≥ 0.75 exceed the ejecta transition and grow secularly. To infer Y$_{RM}$, we first subtract the LDV velocities (inset a) in front of the kh_o^- = 0.35 perturbation (red solid line) for V_{Sp} +U and the flats (black) for U to obtain the net spike growth rate (red dash) V_{Sp}. (This parallels our simulations with and without perturbations to discern bubbles and spikes.) The peak spike growth rate V_{Sp}^o ~ 0.59 ± 0.02 km/s is 40% larger than $\left|V_{MB}\right|$ ~ 0.43 km/s perhaps due to the spike acceleration by the harmonics [1, 12]. We then integrate kV_{Sp} (inset b) to obtain the net scaled spike growth $kh_{Sp}^{max} - kh_o^+$ ~ 1.85 relative to its initial post-shock initial amplitude kh_o^+ ~ −0.29 . (Negative due to opposite phase as in Figs. 1-2). Thus, the saturated spike amplitude is

$kh_{Sp}^{\max} \sim 1.56$. Inserting V_{Sp}^{o} and $kh_{Sp}^{\max}$ into Eq. 3, we obtain an average Y_{RM} of 0.47 ± 0.1 GPa over a strain of 0 to $kh_{Sp}^{\max}$. This agrees with the shear stress Y ~0.57 and 0.5 GPa from refs. [7 and 17], respectively, for SR ~ 1-10 μs^{-1}. Similarly, we analyzed the case for $k h_{o}^{-} = 0.12$ where LDV gives a peak $V_{Sp}^{o} \sim 0.13 \pm 0.02$ km/s $\sim 0.85|V_{MB}|$ and $kh_{Sp}^{\max} - kh_{o}^{+} \sim 0.17 \pm 0.03$ upon integration. With $kh_{o}^{+} \sim -0.09$, we insert $kh_{Sp}^{\max} \sim 0.08 \pm 0.03$ and V_{Sp}^{o} into Eq. 3 to obtain $Y_{RM} \sim 0.4 \pm 0.2$ GPa. This is consistent with the result at $k h_{o}^{-} = 0.35$, but the relative uncertainty is larger due to the weaker RMI response at smaller amplitude. Thus, the precision for Y_{RM} can be improved by varying $k h_{o}^{-}$ in finer increments to obtain $|kh_{o}^{+}| << kh_{Sp}^{\max} < 2.5$ and $V_{Sp}^{o} >> 0.02$ km/s (LDV uncertainty).

In summary, we developed a model for the strength suppression of the RMI that can be used to infer yield under shock loading. The model is based on ideal hydrodynamic simulations and corroborated by MD simulations that compare the RMI inferred yield with direct measurements under the same conditions. The model is able to infer the yield of copper in an explosively driven experiment that agrees with previous results. We plan to refine the model and experimental techniques in order to characterize different materials under various shock conditions below and above the ejecta transition. In particular, we note that LDV probes provide a sensitive measure of the RMI, but they apply better to the spikes in front than the bubbles in back. This motivated our formulation of Eqs 1-3 in terms of spikes, especially since bubbles saturate at smaller amplitudes with a more complex dependence on kh_Y.

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Figures

Figure 1: RMI simulations using PAGOSA with Cu (yellow) and gas (black) with Y = 0.5 GPa and u_3 = 2.5 km/s.

Figure 2: Scaled saturation amplitudes for spikes (solid) and bubbles (open) from PAGOSA simulations vs. RMI strength parameter.

Figure 3: Scaled amplitudes and images from SPaSM simulations for u_3 = 1.5 km/s and kh_o^- = 1.

Figure 4: Stress-Strain calculations with SPaSM for Cu conditions in Fig. 3 at T ~ 1000 °K.

Figure 5: RMI experiment with Cu. Top profile shows 4 initial machined perturbations separated by flat regions. pRad images taken at t = 1 μs (top) and 10.1 μs (bottom) relative to shock breakout. LDV probes measure U on flats (black arrows) and U+V_{Sp} in front of perturbations (red arrow) with kh_o^- = 0.35. Inset (a) measured LDV velocities (solid) and spike growth rate V_{Sp} (dashed) in km/s. Inset (b) integral of kV_{Sp} for net spike growth.

$kh_o^- = 0.125$

$\tau = 0$

0.19

2.1

6

0.22

$kh_o^- = 0.18$

1.05

3.7

14

0.65

$kh_o^- = 0.22$

6.4

9.9

$kh_o^- = 0.4$

16.5

X

Z

$k\,h_{Sp}$

$kh_o^- = 0.4$

0.22

0.18

0.125

$k\,h_{Bu}$

0.125

0.18

0.22

$kh_o^- = 0.4$

$\tau \equiv k\left|V_{Bu}^o\right|t$

$kh_o^- = 0.12$

0.75   0.35   1.5

1 µs

10.1 µs

10 mm

(b) $k\int V_{Sp}*dt$

(a) km/s $V_{Sp}+U$ U V_{Sp}

Time (µs)

pRad #426