The effect of microstructure on Rayleigh-Taylor instability growth in solids

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Abstract. The effect that grain size and material processing have on high-strain rate deformation of copper has been assessed through measurements of unstable Rayleigh-Taylor (RT) perturbation growth. The dynamic loading conditions and initial sinusoidal perturbations imposed on the samples are kept constant while the microstructure of the sample material is varied. Different polycrystalline grain-sizes, single-crystal orientations, and strain-hardened samples have all been dynamically tested. The RT perturbation growth is measured by acquiring a time-sequence of radiographs using the Los Alamos National Laboratory Proton Radiography (pRad) Facility. Single-crystal orientation and strain hardening due to material processing are both observed to affect the perturbation growth. However, polycrystalline grain size variations in copper samples do not influence the growth rate under the loading conditions investigated.

1. Introduction
Constitutive strength models have been developed to describe the plastic deformation of metals over large ranges of strain, strain-rate, and temperature. These models provide a mechanism to investigate and predict the behavior of metals in a wide range of industrial, engineering, and defense applications when implemented in large-scale hydrodynamic simulations. Although it has long been recognized that microscopic processes influence the continuum-level plastic deformation of metals, strength models that fully capture such detail do not yet exist. Instead one class of strength model is purely empirical in construction and a direct fit to existing data. Examples of empirical models include the Steinberg-Guinan [1] and Johnson-Cook [2] models. A second category of constitutive strength models, such as the Preston-Tonks-Wallace (PTW) [3], Zerrilli-Armstrong [4], Mechanical Threshold Stress (MTS) [5] models, are more physics-based in construction but inherently limited by the range of conditions over which the materials have been experimentally tested for model parameterization.

Strength model parameters are obtained by fitting stress-strain data acquired primarily from quasi-static load frames and Hopkinson bar experiments. Generally speaking, these experimental techniques yield data at strains of <100%, strain-rates up to 10^4 s^{-1}, and temperatures ranging between 77-900 K. These experimental conditions span those encountered in most industrial and engineering applications and, as such, the strength models can be employed in a predictive capacity so long as they obtain good fits to the data. However, the major predictive uncertainty of the models lies in the range of strain and strain-rate conditions where these experimental techniques are not well suited to yield data. These
conditions, with strains up to several hundred percent at strain-rates between $10^3$ and $10^8$ s$^{-1}$, are precisely the conditions commonly achieved under explosive-loading or high-velocity impact of metals.

Constitutive strength models express the yield strength ($Y$) in terms of internal state variables such as the strain-rate ($\dot{\varepsilon}$), pressure ($P$), temperature ($T$), and potentially numerous “structure” factors ($S$):

$$Y = f(\dot{\varepsilon}, P, T, S_1, S_2, S_3, \ldots)$$  \hspace{1cm} (1)

The structure factors are used to invoke the effects of microstructural features such as dislocations, defects, grain-size, etc. at the continuum-level. Strain ($\varepsilon$) is, strictly speaking, not an internal state variable in the constitutive equation because it is path-dependent and depends on the deformation history of the material. This is clearly demonstrated in Hopkinson-bar tests performed at different rates where the material state is not unique for a given strain [5]. Various constitutive strength models account for strain differently. The PTW model neglects path dependence and introduces an approximate state variable termed the “equivalent plastic strain” by noting that such an approach is reasonable at moderate strain rates ($10^1$-$10^3$ s$^{-1}$). Alternatively, the MTS model evolves the structure functions via a hardening rule as a function of strain. Material anisotropy is generally unaccounted for in strength models with the short-range anisotropy associated with dislocations captured only through the shear modulus. Grain alignment or texture (long-range anisotropy) effects are not typically included in the constitutive strength models either.

Because the strength models are extrapolating beyond available data to conditions of high-strain (>100%) and strain-rate (>10$^4$ s$^{-1}$) and many microscopic processes are not completely accounted for in the continuum models, a series of experiments have been conducted to investigate ways of improving strength models in these extreme deformation conditions. The high-strain and strain-rate conditions are generated utilizing Rayleigh-Taylor instability growth in solid metals. The initial state of the metals is controlled to adjust grain size, grain orientation, and initial strain. The experimental results described here are largely exploratory in nature and intended to identify where sensitivities, and hence potential deficiencies in the constitutive models, exist under such physical conditions.

2. Experiment Description
Rayleigh-Taylor (RT) instabilities occur at interfaces between lower- and higher-density fluids when the lower density fluid accelerates the interface [6]. If the high-density material is not liquid but instead is solid, then RT instabilities can occur with the strength of the solid stabilizing or reducing the perturbation growth [7-9]. Measurements of RT instability growth in solid metals have been used extensively to assess the dynamic strength of solid metals with lasers [10], pulsed power [11], and high explosives (HE) providing the acceleration. Barnes was the first researcher to utilize HE by-products as the low-density fluid to shocklessly accelerate the solid sample [12]. More recently, Raevsky has significantly refined and advanced the technique [13].

The Barnes technique utilizes a metal plate with perturbations of known wavelength and amplitude machined into one side. A small, well defined, vacuum gap exists between the sample plate and a piece of HE. The high explosive is plane-wave initiated with the detonation direction perpendicular to the perturbed sample surface. The HE by-products propagate across the vacuum gap, stagnate on the metal plate, quasi-isentropically increase the pressure at the interface, and shocklessly accelerate the sample. This sample loading technique has been demonstrated to generate pressures in the metal sample up to 80 GPa with strain-rates ranging between $10^4$ and $10^9$ s$^{-1}$ [13]. A schematic of this experimental arrangement is shown in figure 1a.
Figure 1. (a) Schematic illustrating the experimental setup for strength inhibited R-T growth experiments where the low density “fluid” accelerating the sample are high-explosive by-products. (b) Target geometry used for the R-T growth experiments. (c) Schematic of the apparatus used to execute the experiments inside the LANSCE proton radiography facility.

The experimental apparatus, shown in figure 1c, utilizes a 56 mm diameter plane wave HE lens (P56) consisting of PBX 9501 (fast component) and TNT (slow component) with the TNT by-products used to accelerate the sample [14]. The plane-wave HE drive is utilized to keep the experiment acceleration one-dimensional during the early stages of the perturbation growth. The sample is mechanically held a predefined distance from, and parallel to, the output face of the P56 lens. This vacuum gap distance is adjusted to control the sample acceleration and, hence, the RT instability growth.

Although the material processing differs for each sample tested (as discussed in subsequent sections), the target geometry and machining procedure remain constant. The targets, shown in figure 1b, are 31.75 mm in diameter and 1.5 mm thick from the peak of the perturbations to the back surface of the sample. The sinusoidal perturbations are imposed on the front surface of the sample using a submerged wire EDM (electrical discharge machining). These perturbations are 2.0 mm in wavelength with initial amplitudes adjusted between 35-70 μm (70-110 μm peak-to-trough), depending on the anticipated acceleration and material type. Post-fabrication metrology of the surface is used to measure the as-built initial perturbation with typical wavelength deviations of ±0.004 mm and typical amplitude variations of ±0.003 mm. Test samples have been sectioned and subjected to metallurgical examination after fabrication. This analysis reveals a recrystallization layer of ~5 μm (≪bulk grain size) due to the EDM machining. Given the thickness of this surface layer relative to the initial perturbation amplitude and total sample thickness, this recrystallization layer represents only a small volume fraction of the material being tested. A ~7° bevel is imposed on the front surface of the sample thereby leaving only ~20 mm of the front surface with perturbations. The bevel ensures that the sample is thinner at the sample edges than the center and thereby minimizes dynamic sample cupping due to small variations in radial pressure, particularly late in the experiment. The radial pressure variation occurs because HE by-products expand radially as well as axially as they cross the vacuum gap. If significant cupping of the sample occurs, then the edges of the sample begin to radiographically obscure the bottoms of the perturbations as the sample dynamically deforms.

The sample acceleration is measured at the back or free surface (i.e. the side away from the perturbations) during every experiment using Photonic Doppler Velocimetry (PDV) [15]. Collimated
optical PDV probes typically track the velocity for 4-5 μs before being obscured by fast-moving (~10 km/s) HE by-products. These velocity measurements (see figure 2) provide an essential constraint on hydrodynamic simulations of the experiments as the vacuum gap distance is varied. They are also used to verify shockless acceleration and experiment-to-experiment repeatability.

![Figure 2](image)

**Figure 2.** A representative set of PDV free-surface velocity (mm/μs) measurements vs. time (μs) obtained from the single-stage drive system illustrates acceleration reproducibility, shockless loading, and variations with vacuum gap distance.

The perturbation amplitude is measured at a sequence of discrete times using proton radiography. The Proton Radiography facility (pRad) uses the 800 MeV proton beam from the Los Alamos Neutron Science Center (LANSCE) accelerator to interrogate and image dynamic experiments [16]. The radiograph interframe time is typically chosen to be from 350-500 ns with an integration time of 60-80 ns. The ×3 magnifier provides a 40 mm × 40 mm field-of-view with the target traversing the central 15-20 mm during a typical experiment. Up to 39 total radiographs are acquired during an experiment with most of the data coming from 19 high-resolution images acquired at imaging station 1. These images provide ~100 μm spatial resolution of the perturbations edges. However, chromatic aberrations can degrade the resolution for both the earliest and latest images due to the time-varying HE by-product density.

A typical proton radiograph data set acquired for an annealed copper sample is shown in figure 3. The single stage HE drive system is below the field-of-view in each image. The HE by-products initially reach the sample across the vacuum gap at T₀ +6.9 μs, where T₀ is the initiation time of the detonator on the P56 HE lens. The sample is accelerating upward in each image with the perturbations growing opposite the acceleration direction. Small tubular shrouds surrounding the PDV probes are visible at the top edge of the images. These shrouds delay PDV probe obscuration by the fast HE by-products for a few microseconds.

It is essential to ensure the perturbations initially imposed on the target are precisely aligned with the proton beam axis. As such, the experimental assembly has provisions to tip, tilt, and rotate both the sample and HE. Steel alignment pins used to verify rotational alignment are visible at the left edge of each image in figure 3. These pins are located upstream and downstream (i.e. along the axis of the proton beam) of the object plane.

### 3. Experimental Results

The RT instability growth technique has been used to experimentally investigate the influence of microstructure on high strain-rate strength using four different copper sample types: fully annealed, strain-hardened, a range of average grain sizes, and single-crystals. Although these data are frequently compared against hydrodynamic simulations using different strength models, the discussion here focuses on RT growth comparisons between the different sample microstructures.
Figure 3. A sequence of nine transmission radiographs measuring the perturbation growth in annealed Cu with a 60 μm average grain size. $T_0$ is defined as the initiation time of the detonator attached to the plane-wave HE lens.

3.1. Strain Hardened Copper

It is well known that strain-hardening can significantly alter the stress-strain response of copper at low to moderate strain rates. Strain hardening occurs because dislocations are produced (either dynamically or quasi-statically) within the sample. It is the motion of these dislocations through the material that governs the dynamic strength. Because thermally assisted dislocation glide is the physical mechanism allowing dislocations to move past one another, increased dislocation density at a constant temperature increases the material resistance to plastic flow at intermediate ($10^1$-$10^4$ s$^{-1}$) strain-rates. However, at high strain-rates thermal processes become less important and the dominant mechanism becomes one of dislocation drag [17]. Since high-rate regimes can be accessed with the RT growth technique, it provides a useful way to assess sensitivities to initial material processing under such conditions.

A comparison has been made between the RT growth of perturbations in fully characterized, annealed copper and strain-hardened copper of identical pedigree. The strain-hardened copper samples were obtained via a 30% rolling reduction process. Post-processing metallurgical analysis reveals an elongated grain structure with both annealing twins and a high slip band density.

Four samples were manufactured and tested with the single-stage drive system using a 3.0 mm vacuum gap. Two of the samples were fabricated from fully annealed copper and had an initial amplitude of $A_0 = 55$ μm and 35 μm (110 μm and 70 μm peak-to-trough, respectively). The other two samples were fabricated from the strain-hardened copper with identical initial perturbation amplitudes.

The measured RT perturbation growth for the two different sample types is shown in figure 4a. The strain-hardened material exhibits much higher dynamic yield strength than the annealed samples. The $A_0 = 55$ μm (110 μm peak-to-trough) annealed sample growth rate is 3.3 times the strain-hardened material. The $A_0 = 35$ μm (70 μm peak-to-trough) strain-hardened material completely stabilizes the RT perturbations unlike the annealed sample which undergoes unstable growth.
Figure 4. RT growth data all acquired using identical HE drive systems and a 3.0 mm vacuum gap. (a) Extracted perturbation amplitudes for annealed and strain-hardened copper samples. The growth rate for $A_0 = 55 \mu m$ annealed copper is 3.3 times higher than for pre-strained samples. (b) Perturbation amplitudes extracted from sequences of proton radiographs for 60 $\mu m$, 100 $\mu m$, and 200 $\mu m$ average grain size samples copper samples.

3.2. Grain size variation

Another microstructural phenomena known to increase the yield strength of a metal is grain boundary strengthening (also known as Hall-Petch strengthening) [18]. Grain boundary strengthening occurs because dislocation motion through the material is impeded by grain boundaries that act as pinning points. Dislocations become pinned at boundaries because the change in crystallographic orientation between grains poses a small energy barrier to dislocation motion. As a result, dislocations tend to “pile up” at the grain boundaries with the impeded dislocation motion causing a net increase in yield strength. Hence, smaller grain sizes increase the yield strength of a metal due to the increased number of pinning points and larger grain sizes decrease the yield strength. Grain boundary strengthening has been experimentally demonstrated in samples with grain sizes ranging between 1-1000 $\mu m$ under strain-rate conditions below $10^4$ s$^{-1}$ [19]. It is important to note materials with extremely small grain sizes (<100 nm) do not continue to strengthen, but instead saturate or even begin to weaken. This phenomenon is commonly referred to as the inverse Hall-Petch effect.

The tested copper samples were fabricated from material with three different average grain sizes: 60 $\mu m$, 100 $\mu m$, and 200 $\mu m$. Each sample type originated from the same material lot of half-hard copper, but subjected to different heat treatments. The 60 $\mu m$ average grain size material is the standard, “fully annealed” Cu subjected to a vacuum heat treatment of 600 °C for 1 hour. The 100 $\mu m$ and 200 $\mu m$ grain size Cu samples were vacuum heat treated at 850 °C for 1 hour and 900 °C for 30 minutes, respectively. Idential sinusoidal perturbations were imposed on the samples with an initial amplitude $A_0 = 55 \mu m$ (110 $\mu m$ peak-to-trough). Each Cu sample type was experimentally tested using the single-stage drive system with a 3.0 mm vacuum gap.

The perturbation amplitudes extracted for the three different grain size copper samples are shown in figure 4b. There is no measureable difference in perturbation growth over a 150 $\mu m$ range in average grain size. These data indicate that grain boundary strengthening is not a significant contributor to dynamic yield strength at strain rates above $10^5$ s$^{-1}$ for samples with grains in the range of ~10-100 $\mu m$ average size.

3.3. Single Crystal Copper

Predicting the response of polycrystalline materials consisting of many grains and dislocations (both intra- and inter-granular) is the intent of continuum level strength models. These models do not generally account for anisotropy or crystalline orientation. However, preferred slip planes for dislocation motion do exist within single crystals and, combined with preferred slip directions within
these planes, they constitute a slip system. Face centered cubic materials such as copper have four slip planes {111} and three slip directions <110> for a total of 12 slip systems.

The RT perturbation growth technique was utilized to isolate the role that crystalline slip has on the bulk yield strength of a material. Slip systems are activated through shear and the shear is lowest parallel to the sinusoidal peaks and troughs for an evolving sinusoidal perturbation. Therefore, keeping the acceleration direction constant and changing the orientation of the imposed perturbations relative to the crystallographic axes can preferentially activate different Cu slip systems.

Single crystal RT growth samples 19.0 mm in diameter were fabricated from a large single crystal of copper (approximately 20 mm × 20 mm × 70 mm). Each sample was interference fit into a beveled ring to replicate the sample geometry previously discussed. Two single crystal samples were fabricated and accelerated along the <001> direction with the peaks and troughs of the sinusoidal perturbations parallel to the <100> and <011> directions (See figure 5). Each sample type was experimentally tested using the single-stage drive system with a 3.0 mm vacuum gap.

Figure 5. Proton radiographs of single crystal RT growth experiments acquired at the same times relative to detonator initiation are shown. The growth factor for perturbations oriented in the <100> direction (a) is only 80% of those oriented in the <011> direction (b).

Two of the single crystal copper proton radiographs acquired at identical times are shown in figure 5. The measured growth factor for the sample with the perturbations oriented along the <011> direction is 1.2 times larger than those aligned along the <001> direction. This trend toward lower dynamic material strength is consistent with theoretical expectations because the shear caused by sinusoids oriented along the <011> activates more slip systems in the FCC lattice. Additional, experiments are needed to investigate if single crystal strength is also sensitive to the acceleration direction.

4. Conclusions
The effect that grain size, crystalline orientation, and material processing have on high-strain rate deformation of copper has been assessed through measurements of unstable Rayleigh-Taylor (RT) perturbation growth. In order to isolate microstructural sensitivities of high rate dynamic strength, the dynamic loading conditions and initial perturbations imposed on the samples were kept constant while
varying the sample material. Different polycrystalline grain-sizes, single-crystal, and strain-hardened samples were dynamically tested with the RT perturbation growth measured via a time-sequence of proton radiographs. The crystallographic orientation of single-crystals is observed to affect the perturbation growth in a manner consistent with activation of available slip systems. Stain hardening significantly increases the dynamic strength of materials at strain-rates above $10^5$ s$^{-1}$. Constitutive strength model improvements for use in hydrodynamic simulations need to include these microstructural effects in order to be predictive for high-strain and strain-rate applications. Grain boundary strengthening is not observed to influence the RT perturbation growth rate for copper over the range of conditions and grain sizes investigated.

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