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SCALING, MICROSTRUCTURE AND DYNAMIC FRACTURE

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Abstract. The relationship between pullback velocity and impact velocity is studied for different microstructures in Cu. A size distribution of potential nucleation sites is derived under the conditions of an applied stochastic stress field. The size distribution depends on flow stress leading to a connection between the plastic flow appropriate to a given microstructure and nucleation rate. The pullback velocity in turn depends on the nucleation rate resulting in a prediction for the relationship between pullback velocity and flow stress. The theory is compared to observations of Cu on Cu gas-gun experiments (10 - 50 GPa) for a diverse set of microstructures. The scaling law is incorporated into a 1D finite difference code and is shown to reproduce the experimental data with one adjustable parameter that depends only on a nucleation exponent, Γ.

Keywords: Spall, plastic flow, Langevin equation, nucleation, fracture.
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INTRODUCTION

The dynamic failure of metals under tension is understood to involve the nucleation and growth of microvoids. In addition, the initial as well as shock induced microstructure of the metal can significantly affect its damage evolution and corresponding dynamic strength. Our goal is to understand the role of microstructure in the nucleation and growth process and put it on a more quantitative basis. A self-consistent quantitative theory is introduced that agrees well with a number of experimental observations [1,2]. The centerpiece of the quantitative theory is the size distribution of microvoids either induced or preexisting in the stressed metal. In particular, a microvoid size distribution is derived and shown to depend on the average driving stress and the magnitude of the stochastic noise in the applied stress field. The stochastic stress field in turn depends on the microstructure through the flow stress. One of the interesting results is that the pullback velocity depends mainly on the magnitude of the flow stress even if the microstructural origin of the flow stress may be significantly different [2].

EXPERIMENT

The theory presented here was guided by the results from a suite of Cu on Cu gas-gun experiments described in detail elsewhere [1, 2]. The controls in the experiments were the Cu impact velocity and the initial microstructure of the Cu target. The range of impact velocities corresponding to a shock pressure range of 10 - 50 GPa were chosen to be significantly higher than the characteristic threshold for spall ~ 1 GPa. The microstructures for the Cu target were chosen to study the sensitivity to microvoid nucleation in the pressure range of interest. Single crystals free of grain boundaries typically have larger pullback velocities than polycrystals and this is also observed in these experiments. In addition, the presence of other types of defects incorporated into the Cu crystals will serve as a potent source of nucleation sites and significantly alter the stress threshold for dynamic failure of the Cu. The logarithmic sensitivity of the pullback velocity to impact pressure is observed to be different for the different microstructures Fig. 1. We define an exponent α to describe the observed scaling between impact velocity v_I and pullback velocity v_{pb}

$$v_{pb} \sim v_I^{\alpha} \tag{1}$$

The slope, α, increases with grain size and approaches the highest value of ~1/2 for the single crystal case. In the following we discuss the possible origin of the power law scaling in terms of nucleation and suggest an inverse relationship between α and the flow stress of a particular microstructure.

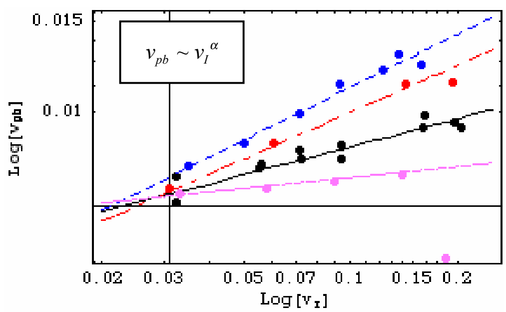

Figure 1. Logarithmic plot of pullback velocity v_{pb} versus impact velocity v_I for a.) Cu 111 single crystal (dashed line), b.) Cu 50 μm grain size (dash-dot-dash), c.) Cu 8.6 μm grain size (solid line) and d.) Cu 100 single crystal+1.5 wt% Si (dotted line).

THEORY

Scaling of Pullback Velocity with Pressure

The pullback velocity observed in the VISAR record of the free surface particle velocity is the result of the dynamic response of the material to tensile loading. It is widely understood that it is not an intrinsic property of the material, but a consequence of time dependent nonlinear and nonequilibrium processes. The pullback velocity is known to depend on both the nucleation rate and the duration over which the applied tensile stress can do the work necessary to create new void volume. In order to derive a scaling exponent relating v_{pb} to [redacted] in terms of nucleation and growth. The void fraction Φ at time t may be approximated as

$$\Phi(t) \propto J(\sigma_I) \int_{t(\sigma_0)}^{t(\sigma_{pb})} d\tau \left[\sigma(\tau) - \sigma_0\right]^{\lambda} \tag{2}$$

The nucleation rate $J(\sigma_I)$ represents the number of voids per unit volume for a given impact velocity that subsequently grow at a rate proportional to the applied tensile stress. The exponent λ takes into account the renormalized stress that a growing void sees in the self-consistent field of other voids. Typically, 1 < λ < 2 [3] and in the present Cu experiments λ =1. The nucleation rate is assumed in the following to be determined prior to the tensile loading at the spall plane, hence is taken to represent a stationary distribution of nucleation sites for a given shock stress σ_I. If it is further assumed for the purposes of scaling that the tensile loading rate is, & then the value of the tensile stress when the void fraction reaches a critical (e.g. percolation theory) value Φ_c is

$$\sigma(\Phi_c) \sim \left[\frac{\sigma}{J(\sigma)}\right]^{\frac{1}{1+\lambda}} \tag{3}$$

The required scaling is obtained once the following identifications are made,

$$J(\sigma_I) \sim \sigma_I^{\Gamma} \qquad \& \sim \sigma_I \tag{4}$$

Finally, since the shock stress is proportional to the impact velocity and the tensile stress at the percolation fraction is proportional to the pullback velocity, the desired result is,

$$v_{pb} \sim v_I^{\alpha} \qquad \alpha = \frac{1-\Gamma}{1+\lambda} \tag{5}$$

The exponent α depends on how the nucleation rate increases with shock stress and the strain rate dependence of the tensile loading which also tends to decrease the time duration over which the tensile load can act. It is widely observed [4] in general that the nucleation rate increases with shock pressure. In the next section the nucleation exponent Γ will be derived for a stationary distribution of microvoids generated in a stochastic stress field which depends on the shock stress and stress fluctuations that depend on the microstructural environment.

Size Distributions and the Nucleation Exponent Γ

The nucleation rate may be estimated from the free energy barriers of a given size cluster, droplet, or in this case void. The free energy barrier depends on the length scale as a result of competing surface and volume contributions. This leads to a characteristic pressure at which microvoids may be activated. Different size distributions can lead to very different nucleation rates for the same tensile loading conditions. Here, we derive size distribution due to the stochastic growth of a microvoid in a fluctuating stress field and with a size dependent threshold stress, $\tau_0 f(\xi)$,

$$\dot{\xi} = \langle \tau \rangle \xi - \tau_0 f(\xi)\xi + \delta\tau(t)\xi \qquad (6)$$

The Langevin equation describes the stochastic change in size under the influence of an average applied stress <τ> and a Gaussian multiplicative noise term δτ(t) and satisfies the correlation relation

$$\langle \delta\tau(0)\delta\tau(t) \rangle = Q\,\delta(t) \qquad (7)$$

. The dimensionless function $f(\xi)$ represents the size dependence of the threshold stress. The Langevin Equation may be mapped onto a time dependent Fokker-Planck Equation for the evolution of the size distribution [5]. The resulting stationary size distribution is

$$N(\xi) = N_0\, \xi^{-1+\frac{2\langle\tau\rangle}{Q}}\, e^{-\frac{2\tau_0}{Q}\int \frac{f(\xi)}{\xi} d\xi} \qquad (8)$$

This distribution is a scale invariant power law modulated by an exponential size cutoff depending on the details of the size dependent threshold. In general, the distribution is peaked and approximates a lognormal distribution for $f(\xi) \sim \xi^{\gamma}$. In the case that $2\langle\tau\rangle/Q < 1$, the distribution is monotonically decreasing and for $\tau_0 << Q$, the power-law dominates

$$N(\xi) \approx \xi^{-1+\frac{2\langle\tau\rangle}{Q}} \qquad (9)$$

The magnitude of the stress fluctuations determines not only the slope but the extent of the power law, consequently higher values of Q lead to a higher tail in the size distribution and a greater probability that a critical size will rapidly grow for the same applied stress.
Nucleation theory provides a connection between the length scale of a droplet, cluster or void, the droplet free energy and the nucleation rate [6]. The free energy for an arbitrary void of l atoms depends on temperature and stress

$$F(l) = a_V(\sigma) l - a_S(T) l^{\sigma_p} \qquad (10)$$

where only the volume and surface contributions to the free energy have been included. The exponent, σ_p, characterizes the surface and $\sigma_p = 2/3$ for a nonfractal d=3 sphere. The nucleation rate is a maximum for a value of l that minimizes the free energy barrier

$$\frac{dF(l_c)}{dl} = 0 \qquad l = \left[\frac{\sigma_p a_S(T)}{a_V(\sigma_c)}\right]^{\frac{1}{1-\sigma_p}} \qquad (11)$$

The relationship between the critical size and the critical stress [6] for irregularly shaped microvoids may be summarized in terms of a single scaling exponent y,

$$\xi_c \sim \sigma_c^{-y} \quad (12)$$

The exponent y depends on the physical system at hand, e.g. cavitation in liquids versus solids where the elastic energy plays an important role. The nucleation rate is sharply peaked at the value of ξ_c and therefore the value of σ_c that minimizes the free energy, i.e.

$$J(\sigma_c) \propto N(\sigma_c(\xi_c)) \sim \sigma_c^{-y\left(-1+\frac{2\langle\tau\rangle}{Q}\right)} \quad (13)$$

which leads to the following identifications

$$\Gamma = y\left(1-\frac{2\langle\tau\rangle}{Q}\right) \qquad \alpha = \frac{1-y+y\frac{2\langle\tau\rangle}{Q}}{1+\lambda} \quad (14)$$

The value of y for d=2 and 3, is bracketed and takes on a value of $y \approx 1$, which results in a simple inverse relationship $\alpha : Q^{-1}$. Furthermore, this leads to the general result that the logarithmic slope of the pullback velocity with impact velocity decreases with the magnitude of the stress fluctuations. If, in addition, the magnitude of Q is proportional to the flow stress $\hat{\sigma}$, then the value of α will saturate with increasing grain size λ_G. This may be understood in terms of the Hall-Petch relationship for polycrystals, which states that

$$\hat{\sigma} = \hat{\sigma}_0 + \frac{k}{\sqrt{\lambda_G}} \quad (15)$$

An interesting consequence of the foregoing analysis is that the origin of the stress fluctuations and therefore pullback velocity, would be approximately invariant, provided $k/\sqrt{\lambda_G} \approx const.$ Experimental support for this assertion has been provided by Kumar et. al. [2] In particular, Cu samples were engineered with two different microstructures with the same measured flow stress. The gas-gun experiments showed the same pullback velocities for the same flow stress, even though the average grain sizes were significantly different.

CONCLUSIONS

The logarithmic sensitivity of pullback velocity to impact velocity for different microstructures can be understood in terms of the distribution of microvoids generated in a stochastic stress field. The magnitude of the stress fluctuations is proportional to the flow stress, which leads to higher nucleation rates for a given impact velocity. The logarithmic sensitivity is found to be inversely proportional to the flow stress and further tested experimentally with engineered microstructures. The scaling was incorporated into an LLNL [7] 1-D finite element code and reproduces the observed pullback velocities from 10-50 GPa, once the nucleation exponent Γ is specified.

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