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On the ultimate tensile strength of tantalum

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ABSTRACT

Strain rate, temperature, and microstructure play a significant role in the mechanical response of materials. Using non-equilibrium molecular dynamics simulations, we characterize the ductile tensile failure of a model body-centered cubic metal, tantalum, over six orders of magnitude in strain rate. Molecular dynamics calculations combined with reported experimental measurements show power-law kinetic relationships that vary as a function of dominant defect mechanism and grain size. The maximum sustained tensile stress, or spall strength, increases with increasing strain rate, before ultimately saturating at ultra-high strain rates, i.e. those approaching or exceeding the Debye frequency. The upper limit of tensile strength can be well estimated by the cohesive energy, or the energy required to separate atoms from one another. At strain rates below the Debye frequency, the spall strength of nanocrystalline Ta is less than single crystalline tantalum. This occurs in part due to the decreased flow stress of the grain boundaries; stress concentrations at grain boundaries that arise due to compatibility requirements; and the growing fraction of grain-boundary atoms as grain size is decreased into the nanocrystalline regime. In the present cases, voids nucleate at defect structures present in the microstructure. The exact makeup and distribution of defects is controlled by the initial microstructure and the plastic deformation during both compression and expansion, where grain boundaries and grain orientation play critical roles.

1. Introduction

The tensile strength of metals is determined by the nucleation, growth, and coalescence of voids and/or cracks. At low strain rates, the applied traction generates an internal stress state that is relaxed by the introduction of these defects. As the strain rate is increased, stress-wave propagation becomes gradually more important and the stress state becomes increasingly non-uniform. Concomitantly, the competition between void nucleation, void growth, and wave propagation effects increases the complexity of the process.

The high strain-rate regime is attained in uniaxial strain, a characteristic feature of shock wave propagation, and in a geometry for which the lateral dimensions of the specimen are larger than the pulse length. Tensile failure in this regime is commonly known as "spall" - a process of physical damage evolution that is initiated by a rarefaction wave, or set of waves, whose amplitude exceeds the local tensile strength of the material [1]. Upon exceeding the local tensile strength of a material, ductile voids or brittle cracks nucleate and subsequently grow to relax the stress by dislocation emission, twinning, or displace phase transformations [2]. In addition to the microstructure, the duration and speed of the release dictates void concentration, sizes, and distributions thereof [3]. Voids often grow via dynamic dislocation generation [4] and coalesce into interconnected void volumes that may cause the material to undergo complete failure. If full separation of the material is incomplete, the response is deemed incipient spall. The process of void nucleation, growth, and coalescence is of critical interest in many fields due to the prevalence of spall damage in engineering applications such as ballistic penetration as well as dynamic fragmentation during hypervelocity impact events that occur in near orbit and outer space.

Dynamic fracture was first documented by Hopkinson [5] and has since seen a long history of study using explosives, gas guns, flyer plates, and lasers [1,4,6–14] to induce tensile failure at strain rates ranging from 10^4 to $5 \times 10^9\ s^{-1}$. There is a strong experimental

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and theoretical foundation that shows an increase in spall strength with increasing strain rate [4,7,12,14]. There is also significant evidence that polycrystallinity decreases the spall strength as compared to single crystals [9,15,16]. Christy et al. [17] performed experiments on polycrystalline copper and observed clear differences in the frequency at which voids nucleate at grain/twin boundaries compared to the grain interior for three different grain sizes - rationalized later by Meyers [18] and Meyers and Zurek [19].

State of the art experimental studies use indirect measures (such as free surface velocimetry [11,20] or Laue diffraction [21,22]) to infer the internal stress states of the material during dynamic failure. Although highly useful, these experimental measurement techniques rely on accurate equation of state (EOS) data (which prescribes the shock Hugoniot path) [13,20,23,24] as well as several bulk acoustic assumptions and simplifications that break down for realistic microstructures, high strain rates, or large amounts of plasticity and/or damage evolution [25]. Several studies utilize post-mortem microscopy to identify damage, but it is often difficult to trace damage back to a specific source [15] and the spall strength and damage field are not unique to one another [26]. Other techniques are being developed, such as the use of high speed imaging [27], that may address some of the issues enumerated here. Critically, spall models strongly rely on empirical data [25,28,29] for which many important quantities are often lacking.

Large scale molecular dynamics (MD) simulations have reached equivalent spatial and temporal scales of laser-driven shock experiments and contain complete, time-resolved, atomic-scale resolution of the relevant damage mechanisms [30–32]. Simulations allow for a well-informed evaluation of spall strength at high strain rates and assist in our interpretation of experimental results. The principal aim of this work is to identify void initiation conditions as a function of defect structure and strain rate in order to establish macroscopic properties such as cohesive strength, maximum sustained tensile load, and damage evolution. Under shock compression it was shown that nanocrystalline metals exhibit ultrahigh strength [30] and here we evaluate the strength of single and nanocrystalline metals under tensile release that often follows the compressed state. For the present study, we focus on tantalum, a model body-centered cubic (bcc) metal, for which an embedded atom model (EAM) potential well-suited for shock simulations is applicable [33,34]. The chosen potential is able to reproduce important properties including the shock Hugoniot; properties of defects such as the gamma surface and energies of the twinning/antitwinning paths; and the stress tensor resulting from uniaxial compressive strains [33]. The potential was also fit to the DFT cold curve of Ta up to 50% volumetric expansion [33]. Details of the elastic properties under tensile stress are provided in the Supplemental Material. There exist a number of important MD studies evaluating spall in model systems [35], Cu [16,36–39], Ni [40], Fe [41], and Ta [42–45] plus several studies that evaluate the dynamics of void growth and defect emission [46–49].

Critical findings of these prior studies identify that free surface velocimetry based calculations underestimate the strain rate and can significantly overestimate the spall strength for Taylor waves (shock waves with a dispersive tail) [37]. It is suggested that corrections to the bulk sound speed and bulk density need to be taken into account to accurately represent the damaged state; this was remarked on earlier by Chen et al. [25] when considering the validity of estimating spall strength by traditional measurements. Multiple studies suggest that under strong shock conditions the resulting defect structures created during compression may overshadow pre-existing defects and thus the initial microstructure or crystalline orientation plays a limited role during spall failure [36,42,50]. Other studies show that the character of defects present in the original microstructure, such as specific grain boundaries or grain sizes, play a significant role in the observed spall strength of metals [9,15]; Mackenchery et al. [16] explicitly show that an increased twin presence in certain nanocrystalline grain sizes influences the peak tensile stress at which voids nucleate at grain boundaries for face-centered cubic (fcc) Cu.

It has been demonstrated that the high strain rates produced through laser-shock techniques decrease the mean spacing between nucleated voids [3]. Voids continue to nucleate throughout the nucleation-growth-coalescence process [44] and the damage evolution and sustained tensile strength exhibits critical behavior relating to the growth of sufficiently large voids [42]. The growth of voids is kinetically limited by the emission of defects such as twins, dislocations, and plastic flow that depend on the strain rate, size of the void, and the complex stress state around them [48].

Ultimately, we aim to describe the spall strength, σ_{sp}, of tantalum as a function of microstructure, strain rate ($\dot{\varepsilon}$), and temperature (T). We can enumerate a basic formalism that the spall strength is a function of these variables:

$$\sigma_{sp} = f(Z, s, \dot{\varepsilon}, T) < \sigma_{\max}(Z, s), \tag{1}$$

where Z defines the material composition and phases; $\boldsymbol{s}$ is a set of microstructure descriptors, including grain size statistics (mean size, distributions of size and/or shape, etc.), texture, grain boundary and triple junction character, and so forth. The variables in Eq. (1) are intrinsically coupled to one another. For instance, strain rate influences the type and quantity of defects that form, this in turn dictates increases in the local temperature from the heat generated by plastic work as defects move through the lattice, and the resulting temperature adjusts the intrinsic barriers to further dislocation motion. This interconnected series of processes is especially crucial during spallation events where the location of spall failure is highly history dependent. It has been established that void nucleation depends principally on the rate, which stems from the role of time on the connected dislocation processes such as thermally activated or viscous-drag limited motion. Relatedly, increasing the strain rate raises the spall strength of the material, a process that relates the competition between void nucleation and void growth [14,51]. Both processes are intimately tied to dislocations, both nucleation and the subsequent motion thereof, which are effected by the plastic strain rate according to the classical Orowan [52] equation. For strain-rate experiments greater than 10^4 s^{-1}, the spall strength is typically expressed with a power law relationship [12,14]

$$\sigma_{sp} = \sigma_0 (\dot{\varepsilon})^{m_1}. \tag{2}$$

We will expand on these general relationships throughout the manuscript and use them as an underlying foundation upon which to build.

2. Simulation methods

Multiple non-equilibrium molecular dynamics simulation methods are employed to evaluate dynamic tensile failure in the strain-rate space of 10^7 s^{-1}–10^{13} s^{-1}. These results will be benchmarked against density functional theory (DFT) predictions and EOS calculations. Three methodologies are employed, illustrated graphically in Fig. 1, with characteristic snapshots at time 0, 30 ps, and 60 ps. Each simulation archetype offers specific advantages and disadvantages, as we describe next.

2.1. Flyer plate and target

The collision between a flyer plate and a target (Fig. 1(a))