LLNL-JRNL-432827

Application of a Multiscale Model of Tantalum Deformation at Megabar Pressures

R. M. Cavallo, H. Park, N. R. Barton, B. A. Remignton, S. M. Pollaine, S. T. Prisbrey, J. V. Bernier, M. J. May, B. R. Maddox, D. W. Swift, R. C. Becker, R. T. Olson

May 20, 2010

Defense Science Quarterly

Application of a Multiscale Model of Tantalum Deformation at Megabar Pressures

Robert Cavallo, Hye-Sook Park, Nathan Barton, Bruce Remington, Stephen Pollaine, Shon Prisbrey, Joel Bernier, Mark May, Brian Maddox, David Swift and the Materials Integrated Experimental Team (Lawrence Livermore National Laboratory), Rich Becker (Army Research Laboratory) and Russell Olson (Los Alamos National Laboratory)

A new multiscale simulation tool has been developed to model the strength of tantalum under high-pressure dynamic compression. This new model combines simulations at multiple length scales to explain macroscopic properties of materials. Previously known continuum models of material response under load have built upon a mixture of theoretical physics and experimental phenomenology. Experimental data, typically measured at static pressures, are used as a means of calibration to construct models that parameterize the material properties; e.g., yield stress, work hardening, strain-rate dependence, etc. The pressure dependence for most models enters through the shear modulus, which is used to scale the flow stress. When these models are applied to data taken far outside the calibrated regions of phase space (e.g., strain rate or pressure) they often diverge in their predicted behavior of material deformation.

The new multiscale model, developed at Lawrence Livermore National Laboratory, starts with interatomic quantum mechanical potential and is based on the motion and multiplication of dislocations[1]. The basis for the macroscale model is plastic deformation by phonon drag and thermally activated dislocation motion and strain hardening resulting from elastic interactions among dislocations. The dislocation density, ρ, and dislocation velocity, ν, are connected to the plastic strain rate, $\dot{\varepsilon}^{\mathrm{p}}$, via Orowan's equation: $\dot{\varepsilon}^{\mathrm{p}} = \frac{\rho b v}{M}$, where *b* is the Burger's vector, the shear magnitude associated with a dislocation, and *M* is the Taylor factor, which accounts for geometric effects in how slip systems accommodate the deformation. The evolution of the dislocation density and velocity is carried out in the continuum model by parameterized fits to smaller scale simulations, each informed by calculations on smaller length scales down to atomistic dimensions.

We apply this new model for tantalum to two sets of experiments and compare the results with more traditional models. The experiments are based on the Barnes's[2] technique in which a low density material loads against a metal surface containing a pre-imposed rippled pattern. The loaded sample is Rayleigh-Taylor unstable and the rippled amplitudes grow with time. The rate of growth differs depending on the material strength, with stronger materials growing less, even to the point of saturation. One set of experiments was conducted at the pRad facility at LANSCE at Los Alamos National Laboratory in 2007 using high-explosive (HE) driven tantalum samples. The other set of experiments was done at the Omega laser at the Laboratory for Laser Energetics at the University of Rochester, which used high-powered lasers to create plasmas to dynamically compress a rippled tantalum sample (see, e.g., Park et al.[3,4]). The two techniques provide data at different pressures and strain rates: The HE technique drives the samples at around 2 x 10^5 s^{-1} strain rate and pressures near 500 kbar, while the laser technique hits strain rates around 2 x 10^7 s^{-1} and pressures close to 1.4 Mbar.

The most recent laser experiments were conducted in February 2010 and we present a sample of the data in Figure 1, which shows a face-on radiograph at a time of 65 ns after the laser was turned on. From this radiograph, we measure the growth factor which is defined to be the change in amplitude of the ripples relative to their initial amplitude. Figure 2 shows the resulting growth factors along with various model fits. The error bars are typically 20 – 25%. Only the multiscale model predictions match the experimental measurements.

The growth factors via the HE technique are determined from multiple side-on proton radiography images and thus provide a full growth curve per single experiment. A sample growth curve is shown in Figure 3, also with various model fits and error bars estimated at 25%. It should be noted that by 7.5 μs the growth in this sample has exceeded the initial target thickness indicating that localizations not captured in the overall simulation have probably become dominant; i.e., the target is likely breaking up.

Application of the multiscale dislocation dynamics model as implemented in the Ares[5] hydrodynamics code shows excellent agreement with both the pRad and Omega data. We also compare the Steinberg-Lund[6] (SL), Preston-Tonks-Wallace[7] (PTW), and Steinberg-Guinan[8] (SG) models with the data. The PTW and SG models provide good fits to the pRad data but over-predict the growth (underestimate the strength) on the laser platform. The SL model under-predicts the pRad data and over-predicts the Omega data. The excellent agreement of the multiscale model with the data over two orders of magnitude in strain rate and more than a factor of two in pressure lends credibility to the model. We will continue to stress the model by conducting experiments at 5 Mbars and beyond at the National Ignition Facility at LLNL in the near future

This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

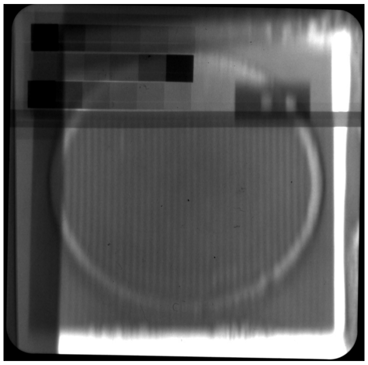

Figure 1: Face-on 22 keV x-ray radiograph of a rippled sample target of tantalum at 65 ns after initial laser pulse. The driven ripples constitute the center of the image, while the upper portion of the image contains added features (stepped filters and knife-edge resolution block) to aid in the extraction of the growth factor. The ripple amplitudes are derived from transmission contrast between peak and valley of the ripple regions.

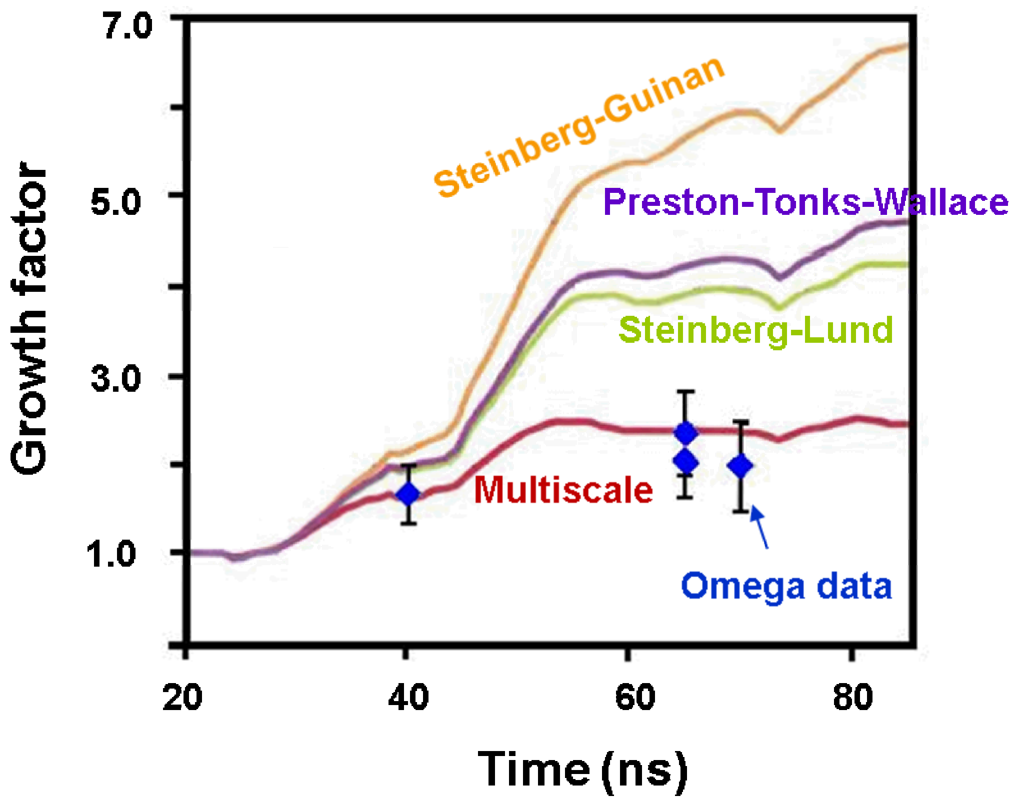

Figure 2: Comparison of various model predictions with growth factor data obtained at the Omega laser facility, Rochester, NY, in 2009 and 2010. The data reach peak pressures between 1.2 and 1.4 Mbar and average strain rates around 2 x 10^7 s^{-1}.

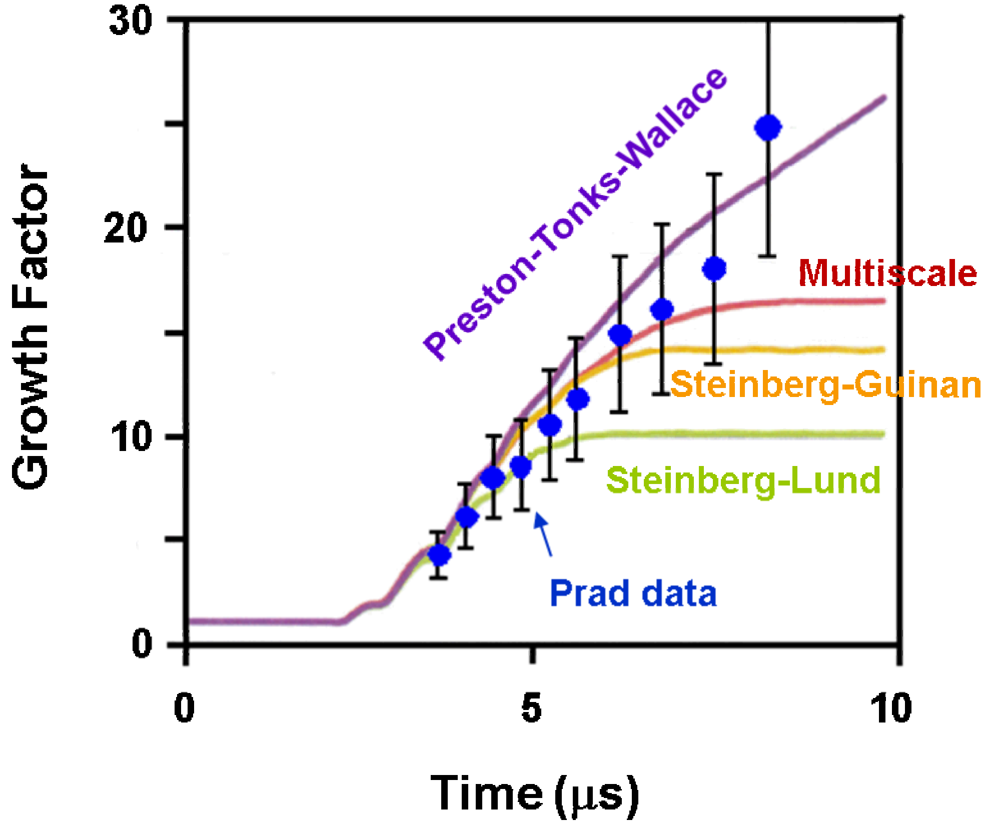

Figure 3: Comparison of various model predictions with growth factor data obtained at the pRad facility, Los Alamos, NM, in 2007. The data reach a peak pressure of 500 kbar and an average strain rate of 2 x 10^5 s^{-1}.

---

[1] Becker, R. et al., A Tantalum Strength Model using Multiscale Approach: Version 2, September 2009, LLNL-TR-417075

[2] J. F. Barnes, P. J. Blewett, R. G. McQueen, K. A. Myer, and D. Vernable, Taylor Instabilities in Solids, J. Appl. Phys. 45, 727 (1974)

[3] H.-S. Park, et al., Viscous Rayleigh-Taylor Instability Experiments at High Pressure and Strain Rate, Phys. Rev. Lett. 104, 135504 (2010)

[4] H.-S. Park, et al., Strong Stabilization of the Rayleigh-Taylor Instability by Material Strength at Megabar Pressures, Phys. Plasmas 17, 056314 (2010)

[5] G. Bazan, in Proceedings from the 2nd International Workshop on Laboratory Astrophysics with Intense Lasers, UCRL-ID-131978, ed. B. A. Remington (Livermore, CA: Lawrence Livermore National Laboratory), 42 (1998)

[6] D. J. Steinberg and C. M. Lund, A Constitutive Model for Strain Rates from 10^{-4} to 10^6 s^{-1}, J. Appl. Phys. 65, 1528 (1989)

[7] D. L. Preston, D. L. Tonks, and D. C. Wallace, Model of Plastic Deformation for Extreme Loading Conditions, J. Appl. Phys. 93, 211 (2003)

[8] D. J. Steinberg, S. G. Cochran, and M. W. Guinan, A Constitutive Model for Metals Applicable at High-Strain Rate, J. Appl. Phys. 51, 1498