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Influence of Shockwave Obliquity on Deformation Twin Formation in Ta

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Abstract. Energetic loading subjects a material to a “Taylor wave” (triangular wave) loading profile that experiences an evolving balance of hydrostatic (spherical) and deviatoric stresses. While much has been learned over the past five decades concerning the propensity of deformation twinning in samples shock-loaded using “square-topped” profiles as a function of peak stress, achieved most commonly via flyer plate loading, less is known concerning twinning propensity during non-1-dimensional sweeping detonation wave loading. Systematic small-scale energetically-driven shock loading experiments were conducted on Ta samples shock loaded with PETN that was edge detonated. Deformation twinning was quantified in post-mortem samples as a function of detonation geometry and radial position. In the edge detonated loading geometry examined in this paper, the average volume fraction of deformation twins was observed to drastically increase with increasing shock obliquity. The results of this study are discussed in light of the formation mechanisms of deformation twins, previous literature studies of twinning in shocked materials, and modeling of the effects of shock obliquity on the evolution of the stress tensor during shock loading.

1. INTRODUCTION

A material shock-loaded via direct contact with a high explosive (HE) experiences a complex loading path that evolves both spatially and temporally. Energetic loading subjects a material to a “Taylor wave” (triangular wave) loading profile that experiences an evolving balance of hydrostatic (spherical) and deviatoric stresses[1]. The manifestation of this effect is that directly under the initiation of detonation of an energetic the loading will initially be nominally 1-D with the hydrostatic loading component dominant. A fully developed sweeping detonation wave running along a plate (obliquity > 80 degrees) however will experience a decreased peak hydrostatic shock stress (> factor of two) while the deviatoric shear stresses are increased substantially (two orders of magnitude) for a von Mises material. While much has been learned over the past five decades concerning the propensity of deformation twinning in shock-loaded samples, these studies have focused principally on 1-dimensionally shock loaded samples where the shocks produced “square-topped” profiles as a function of peak stress and were achieved most commonly via flyer plate loading. However, considerably less is known concerning twinning propensity resulting from direct in-contact HE-driven shock loading where a “Taylor-wave” shockwave profile is applied, let alone a sweeping detonation Taylor-wave loading stress path where the applied stress tensor evolves as a function of obliquity.

Twin initiation in materials is known to occur when the externally applied shear stress across the twinning K_1 plane, resolved in the η_1 twin direction reaches some “critical” value[2]. However, the concept of an absolute “critical resolved shear stress”, as proven to operate in the case of slip, for

twinning remains unsupported in the literature[2] due in part to the complexity and requirements for twinning partial dislocation nucleation to form twins. In regards to shock loading, a number of researchers have postulated a critical shock “pressure” rather than shear stress requirement for the onset of twinning in shocked face-centered cubic metals[3]. However, while shock loading exposes materials to intense peak hydrostatic pressures at high strain rates, it is the resolved shear stresses on operative slip and twinning planes that are known to drive plasticity during shock loading[4], not the magnitude of the peak hydrostatic spherical component of the yield surface which dominates in 1-D uniaxial strain shock loading experiments. Linking twinning propensity to planes and directions of maximum shear stress in shock loading is not a new concept and has been validated in shock studies since the earliest seminal studies of C.S. Smith in 1958 [5]. In this work he correlated the angular frequency of deformation twins formed in shock loaded brass and found the maximum to lie at 45 degrees to the applied shock direction. Changes in the twinning propensity in Cu as a function of the applied peak spherical and deviatoric stresses, i.e., as a function of obliquity[6], imposed during shock loading suggest the concept of a “critical twinning pressure” for copper may be only applicable to 1-D shock loading. Further, contradictions in the observed twinning response of tantalum as a function of peak shock stress between 1-D[7] and complex shock loading paths[8] additionally emphasizes the importance of the hydrostatic and deviatoric components imposed during shock processes on twinning propensity.

This study was prompted by recent experiments where tantalum (Ta) samples were shock loaded *via* direct contact with high explosives in a sweeping-wave geometry that was observed to significantly increase the propensity of deformation twinning. The influence of shock obliquity on twin formation in Ta was quantified and thereafter the change in the spherical and deviatoric stresses as a function of obliquity during shock loading was examined *via* modeling.

2. EXPERIMENTAL TECHNIQUES

The tantalum studied in this investigation was commercially pure, triple electron-beam melted and annealed plate, 10.2 mm in thickness obtained from Cabot Corporation. The chemical composition (in wt%) was analyzed to be carbon 10 ppm, oxygen 50 ppm, nitrogen 10 ppm, hydrogen, 5 ppm tungsten, 25 ppm niobium, 25 ppm titanium, 5 ppm, iron 5 ppm, and the balance Ta. The plate was produced from an ingot, which was forged into a billet; this was then annealed, and subsequently cut prior to cross rolling. The plates were straight-rolled in the final finishing passes. Cross rolling of the Ta plate resulted in divergence from the typical straight-rolled texture, from a partial to a nearly continuous γ fiber ($<111>/ND$), along with the virtual extinction of the partial α fiber ($<110>/RD$). The texture was moderately sharp, with the $<111>$ fiber component approximately eight times random. Average grain size of this material was 42 μm .

Systematic small-scale direct energetically-driven shock loading experiments were conducted where Ta samples were shock loaded with pentaerythritol tetranitrate (PETN) using an exploding foil initiator (EFI) or ‘slapper’ to initiate detonation in the PETN pellet. The subsequent interaction of the detonation front with the metal target transmits a shock wave into the target and reflects a shock wave back into the detonation products. The interactions of these shock waves with the materials and the material boundaries dictate the time-varying stress states that cause plastic deformation and thereafter damage evolution and spallation to proceed. Varying the dimensions of the explosive or target discs, or the number and location of the initiation points directly affects the stress state within the metal target. In this paper the PETN was edge-detonated as schematically shown in Figure 1. The PETN explosive pellets were pressed to average densities in the range of 1.50-1.55 g/cc. For the sweeping-wave experiment, an 8mm diameter disc of Ta that was 1-mm thick was shocked *via* direct loading from a 4-mm thick PETN pellet. Once the metal target disc or component is shocked and begins to accelerate, the shock set-up was configured such that the sample then impacts a block of open cell polymer foam where it decelerates to a stop. Foam of a density of 30mg/cc (1.8 lbs./ft³) was found to successfully decelerate the samples without imparting additional damage into the samples.

The specimen was cross-sectioned and prepared for optical metallography and electron backscatter diffraction (EBSD)[9]. Automated EBSD scans were performed at 20 kV in an FEI XL30 FEG-SEM equipped with TSL data acquisition hardware and software. In each white rectangle location shown in Figure 2 three different areas were chosen for EBSD analysis so that the average twin fraction calculated is representative for that region. These regions were orientation mapped with a step size of $0.15 \mu\text{m}$ in a hexagonal grid. EBSD twin identification was accomplished by defining a twin boundary based on an axis-angle misorientation criterion, using a minimum rotation about the direction common to both parent and twin orientations necessary to bring the matrix and twin orientations into coincidence [10].

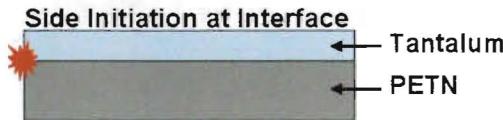


Figure 1. Schematic of side-initiated energetic loading geometry. The exploding foil initiator, explosive pellet and Ta disc were held together by small amounts of glue at the periphery of the cylinders.

3. RESULTS AND DISCUSSION

3.1 Substructure Evolution

The damage and substructure evolution of the shock prestrained Ta as a function of obliquity was examined optically and the types and volume fractions of the deformation twins were quantified using EBSD scans as a function of position within the samples. The 1-D impedance match of the PETN into the Ta is calculated to be nominally 60 GPa, a significant magnitude shock. Optical metallography reveals gradients in the apparent slip band density and propensity for deformation twins as a function of position within the sample, as seen in Figure 2. In response to the sweeping detonation wave, the sample is macroscopically bent and displays a higher density of slip bands and twins near the upper edge in contact with the PETN, as well as ductile fracture at the far end of the sample.

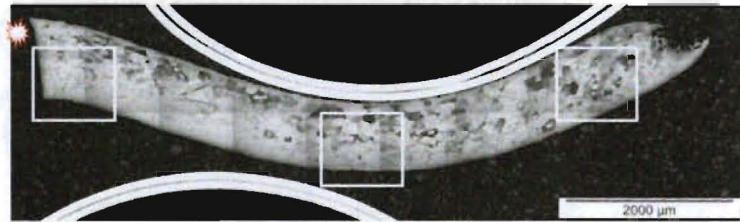


Figure 2. Metallography of PETN-loaded sample showing damage in Ta as a function of position relative to the HE initiation site (denoted with a “star” symbol) for the side interface initiated sample.

The absence of a well-defined spall plane within the side-initiated sample when the peak shock stress is calculated to be ~ 60 GPa is in contrast to 1-D spallation studies on high-purity Ta. In the 1-D spallation samples the spall strength has been documented as only between ~ 5.2 to 6 GPa for square-shaped pulse shock loading[11]. This emphasizes the importance of examining the effects of shock obliquity on defect generation and damage evolution in addition to shock pulse shape and pulse duration on spallation[12].

Quantification of the influence of shock obliquity on deformation twin propensity was conducted using optical metallography and EBSD imaging of the side-initiated Ta sample. Results are presented as a function of position compared to the detonation source as denoted in Figure 2. The optical metallography and EBSD imaging revealed that the density of identifiable twins was

positively correlated with the function of sweep of the detonation wave from the point of initiation in the side-initiated Ta sample. Figure 3 shows optical micrographs and Figure 4 shows the representative EBSD images for the side-initiated shocked sample at fixed magnifications for the three locations. Quantitative analysis of the EBSD images as a function of location was further used to calculate the average twin fraction as presented in Table 1. All the twins observed were of the $K_1 = \{112\}$, $\eta_1 = <111>$ type.



Figure 3. Optical metallography of twins and slip bands in Ta as a function of position relative to the HE side-interface initiated sample. Photos coincident with the left, center, and right locations indicated in Fig. 2.



Figure 4. EBSD maps showing twins in Ta as a function of position relative to the HE initiation site for the side interface initiated sample. Photos coincident with the left, center, and right locations indicated in Fig. 2.

Table 1. Comparison of twin volume fractions as a function of position relative to the HE initiation site for the center face and side edge initiated samples.

	Average Twin Volume Fractions		
	Bottom Left	Bottom Center	Bottom Right
Side interface Initiation	0.21	0.47	0.52

The twin volume fraction increases by over a factor of 2, from the point of detonation across to the far end of the sample where the shock loading has transitioned to a fully developed sweeping detonation wave. The observation of a reasonably modest twin volume fraction adjacent to the PETN initiation site, associated with the peak shock hydrostatic stress, is in stark contrast to previous 1-D square-wave shock loading of high-purity Ta shocked to only 20 GPa which exhibited numerous deformation twins[7]. The current findings of the importance of shockwave obliquity on twinning propensity in Ta are, however, consistent with the previous observations of Sanchez et al. [6], where the obliquity of the shock wave seems to suppress the critical shock pressure for Cu. Sanchez et al. observed twinning at pressures of only 11 GPa in contrast to an established critical twinning pressure of ~20 GPa. Elucidation of the effect of shockwave obliquity on the composition

of the imposed stress tensor (spherical and deviatoric stresses) was examined *via* modeling as described below.

3.2 Modeling of Stress as Function of Wave Obliquity

Consider the interaction of an oblique detonation wave (D) with a PETN/metal interface as depicted by the right-going regular-reflection wave structure of Figure 5a. The wave D propagates into non-reacted HE at an angle of obliquity defined by θ , with D reflecting from the interface as a gas shock S_1 in HE combustion products and a metal shock S_2 . Application of 3D Jump Relationships[13] to each of the three waves in Figure 5a produces a nonlinear set of coupled, algebraic equations (11 equations containing 12 unknowns) involving conservation principles of mass, momentum, energy, Equation-of-State (EOS) and Ta metal flow stress (constitutive) information. The Figure 5a schematic is a two-dimensional (2D) simplification of the more-pragmatic 3D problem. For a specified value of θ (one of the unknowns) the coupled equation set is solved for the stress-strain (or pressure-volume) state in the wake of each wave, and a subset of the results is presented in Figure 5b in terms of stress behind the metal shock S_2 . A nice example of the application of Jump Relationships to the fluids problem depicted in Figure 5a can be found in[14], but note that in the presented work, the metallic region is treated as a solid rather than a fluid such that deviatoric stress can be physically supported and thus computed. Figure 5b presents the pressure and a shear stress component S_{12} (in the plane of the schematic) plotted as a function of obliquity with θ ranging from 0° (a normal wave interaction) to 90° (a so-called sweeping wave interaction); note that the Mach reflection at obliquities in the neighborhood of 55° to 80° is not addressed in this work. The results of Figure 5b show decaying pressure (starting at the Hugoniot pressure), and increasing S_{12} as D wave obliquity increases; the magnitude of S_{12} is consistent with an isotropic yield surface treatment for Ta and starts at zero for normal interaction and then asymptotes to 160 MPa for a sweeping detonation wave. This result quantifies the increasing shear component with position from the edge detonation site in the characterized Ta sample.

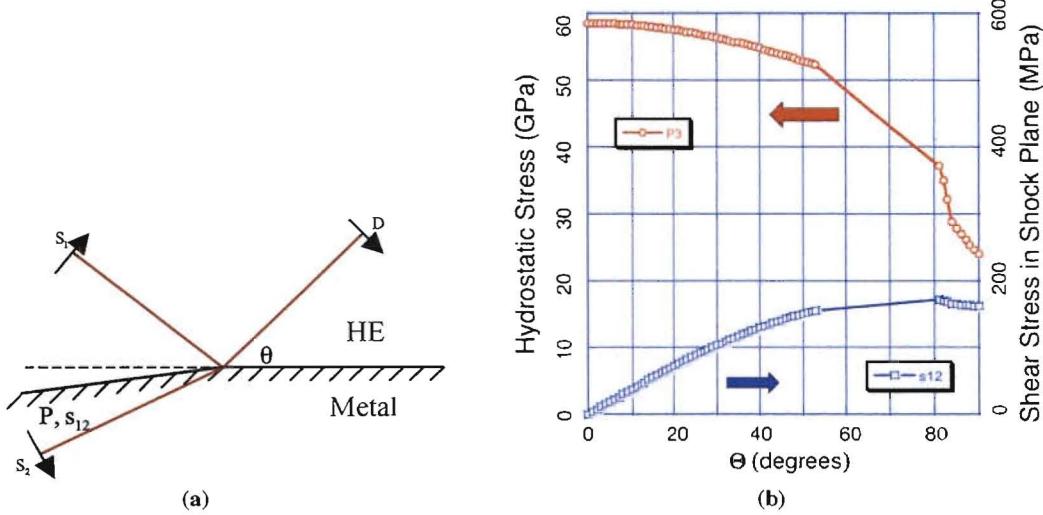


Figure 5. (a): Regular reflection schematic of a detonation wave (D) interaction with a metal surface, and (b): Calculated Hydrostatic (spherical- P_3) and shear (deviatoric- S_{12}) stresses in Ta as a function of D obliquity.

4. SUMMARY AND CONCLUSIONS

The current study of the effect of energetic-driven shock prestraining as a function of shock obliquity on deformation twinning behavior of tantalum (Ta) reveals that:

- 1) Twin formation during shock loading in Ta is seen to be a strong function of shock obliquity, consistent with the effect of obliquity on the imposed stress tensor during shock loading that effectively varies the ratio of the spherical (hydrostatic) and deviatoric (shear) stresses.
- 2) EBSD characterization provides valuable information on twin system activation and twin volume fractions. EBSD results on the Ta as a function of position revealed increasing twin density correlated with greater predicted obliquity.
- 3) Quantification of the effects of shock obliquity on defect generation and damage evolution in shock loaded materials is critical to the development of physically-based models of the shock response of condensed matter.

Acknowledgments

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