Comment on "Strength of Shock-Loaded Single-Crystal Tantalum [100] Determined Using *in situ* Broadband X-Ray Laue Diffraction"

In a recent Letter [1], Comley *et al.* experimentally determine the strength of shock-loaded single-crystal tantalum (Ta) [100] using *in situ* broadband x-ray Laue diffraction. These experimental results are shown to be in excellent agreement with the multiscale strength (MS) model developed by Barton *et al.* [2], but not with traditional strength models, namely, Preston-Tonks-Wallace (PTW) [3], Steinberg-Guinan (SG) [4], and Steinberg-Lund (SL) [5], which are shown to severely underpredict the flow stress. In this Comment, we show that the plastic strain rates used for the model predictions are inconsistent with a key assumption utilized in the determination of the experimental von Mises stresses. If the correct strain rates had been used, all of these strength models would underpredict the von Mises stress, and the experimental measurements would no longer validate the MS model at high pressures and strain rates.

Comley *et al.* use x-ray Laue diffraction to measure the strain state in the compressed Ta single crystal. From the experimental data, they calculate the longitudinal stress, σ_S, and the aspect ratio of the compressed unit cell, α, which is then related to the strain. To determine the von Mises strength, $\bar{\sigma} = 3\sigma_S'/2$, the authors first calculate the deviatoric longitudinal stress, $\sigma_S' = \sigma_S - \bar{P}$, using

$$\sigma_S' = \frac{4}{3} C'(\bar{P}) \Delta\epsilon(\alpha, \eta), \quad (1)$$

where $\bar{P}$ is the shock pressure, $C'(\bar{P}) = [C_{11}(\bar{P}) - C_{12}(\bar{P})]/2$ is the effective shear modulus, and $\Delta\epsilon(\alpha, \eta)$ is a shear strain equal to the difference between the longitudinal strain, ϵ_S, and the transverse strain, ϵ_T, which both depend on the aspect ratio and the compression, η.

Comley *et al.* make the standard assumption that the compressed state lies on the Ta Hugoniot curve. This assumption plays a role in the determination of the longitudinal stress, σ_S, from the experimental data, calculation of the effective shear modulus, $C'(\bar{P})$, from density functional theory (DFT), and finally determination of the compression, η. A fundamental assumption behind the formulation of the Rankine-Hugoniot jump conditions is that the material behind the shock front is in thermodynamic equilibrium [6]. In other words, the shock Hugoniot equation is a locus of equilibrium end states, and provides no information about the material under the dynamic conditions within the shock front. By assuming the compressed state lies on the Ta Hugoniot curve, Comley *et al.* implicitly assume that the system is in equilibrium. Furthermore, since they observe no changes in the strain as a function of time and find no evidence for partially relaxed regions, they conclude that the "material has reached a steady state and nonhydrostatic condition."

All of the strength models considered by Comley *et al.* are strain-rate dependent [2–5]. To correctly compare stresses calculated with these models to the experimentally determined von Mises strengths, the strain rate, $\dot{\epsilon}$, should be set to zero since the compressed state is assumed to lie on the Ta Hugoniot curve, thus in equilibrium with no solid flow. However, Comley *et al.* calculate a strain rate using the Swegle-Grady relation [7]. Interestingly, the strain rate for the steady state compressed material is calculated to be $7.8 \times 10^9\ \mathrm{s}^{-1}$. If the correct strain rate ($\dot{\epsilon} = 0$) had been used, all of the strength model predictions would significantly drop, and the experimental flow stresses would lie far above the predictions of all noted strength models, including the MS model.

We would also like to briefly note some underlying assumptions behind Eq. (1) that impact calculation of σ_S', and hence the flow stress. Specifically, the effective shear modulus, $C'(\bar{P})$, assumes isotropy, but the Zener anisotropy ratio will change with both pressure and temperature, meaning $C'(\bar{P})$ has potential to differ significantly from the shear modulus under these loading conditions [8]. Also, evaluation of $C'(\bar{P})$ on the Hugoniot yields an upper bound rather than an average through the shock. Finally, without including details, we highlight that the α-dependence of $\Delta\epsilon$ given in the text is incorrect in a way that underestimates σ_S'. The magnitude of variation in the flow stress due to these assumptions is not clear but will increase proportionally with compression.

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