Multiple Mechanisms of Thermally Activated Plastic Flow in Shocked and Unshocked Tantalum

William H. Gourdin
David H. Lassila

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PLASTIC FLOW IN SHOCKED AND UNSHOCKED TANTALUM

William H. Gourdin and David H. Lassila
Lawrence Livermore National Laboratory
P.O. Box 808
Livermore, CA 94551
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William H. Gourdin and David H. Lasila
Lawrence Livermore National Laboratory
P.O. Box 808
Livermore, CA 94551

Abstract

We argue that the principal features of the plastic flow behavior of tantalum can be described by a model that incorporates a two-component Peierls-type mechanism and an "obstacle" mechanism in series. We compare the results of calculations based on such a model with flow data for unalloyed tantalum before and after shock loading to 45 GPa for 1.8 ps. Our data suggest that the shock loading changes only structural parameters.

Introduction

As with other body centered cubic (bcc) metals, the mechanical properties of tantalum display marked temperature and strain-rate dependence (1-3). We have suggested (4) that plastic flow in unalloyed tantalum occurs via a series combination of thermally activated mechanisms that dominate the flow in different regimes of deformation, strain rate, and temperature. Because the mechanical threshold associated with at least one of these (the "obstacle" mechanism) increases with deformation, workhardening appears in a natural way. In this paper, we review this concept and its application to shocked and unshocked tantalum.

Model Description

To propagate plastic flow, we propose that a dislocation must overcome a series of barriers, as illustrated schematically in Fig. 1. One type of barrier, represented by the tall peaks in Fig. 1, has a large activation energy, and the stress associated with it increases with increasing deformation (workhardening). We presume that this barrier is produced by intersections of dislocations with other dislocations or dislocation tangles. The second type of barrier, represented by the shorter peaks in Fig. 1, has a small activation energy and has been associated with the intrinsic lattice resistance to dislocation motion (the Peierls barrier) (2). For simplicity of notation, we refer to these two barriers as "obstacle" and "Peierls" barriers, respectively, regardless of their true origin. The total transit time $t_T$ between one obstacle and the next is the sum of the times required to overcome one obstacle and the $n_p$ Peierls barriers in between. Assuming Boltzmann probabilities for overcoming the energy barriers, we thus have

Figure 1. Schematic of two barriers to dislocation motion in series.

$$t_T = \left( \frac{1}{V_o} \right) \exp \left( \frac{G_o}{kT} \right) + \left( \frac{1}{V_p} \right) \exp \left( \frac{G_p}{kT} \right).$$

(1)

where $V_o$ and $V_p$ are the attempt frequencies for each barrier and $G_o$ and $G_p$ are the corresponding activation energies.

The strain rate is proportional to the average dislocation speed $L/t_P$, so that we have

$$\dot{\varepsilon} = \frac{\dot{\varepsilon}_0}{\exp \left( \frac{G_o}{kT} \right) + P \exp \left( \frac{G_p}{kT} \right)},$$

(2)

where $\dot{\varepsilon}_0$ and $P$ are constants suitably defined in terms of $L$, $V_o$, $V_p$, and $n_p$. Equation (2) is the fundamental expression of the model that we propose for unalloyed tantalum."

The flow stress $\sigma$ is frequently written as the sum of a stress $\sigma_o$ associated with thermally activated mechanisms and an "athermal" stress $\sigma_p$ that is affected by temperature only.

* Dislocation drag could easily be included in Eq. (2), but it has little influence under the conditions of our experiments.
through changes in the temperature-dependent shear modulus $\mu(T)$. The Peierls activation energy $G_p$ is a function of the thermal stress $\sigma_T$:

$$\begin{align*}
G_p &= C_p f\left[\frac{\sigma_T}{M(T)\Delta\rho}\right] + C_p^2 \left[1 - \frac{\sigma_T}{M(T)\Delta\rho}\right]^2 \\
&= \tilde{G}_p(\sigma_T) + \tilde{G}_p^2(\sigma_T),
\end{align*}$$

(3)

where the notation $\tilde{G}_p, \tilde{G}_p^2$ is used in Fig. 1. We associate the first ("primary") term with the Peierls energy reported in previous work (2, 3), for which the primary threshold stress $\tilde{\sigma}_p$ does not change with deformation. The function $f$ in the primary term is close to the parabolic forms used elsewhere (2), but deviates from this form at large stresses to accommodate observed behavior at low temperatures and high strain rates. The secondary energy $G_p^2$ and threshold stress $\tilde{\sigma}_p^2$ are selected to agree with available data (1).

The obstacle term in Eq. (2) is treated in a manner identical with that for copper (5, 6). The obstacle activation energy $G_o$ is given by

$$G_o = C_o \left[1 - \frac{\sigma_T}{M(T)\Delta\rho}\right]^p,$$

(4)

The mechanical threshold $\tilde{\sigma}_o$ increases with true strain $\varepsilon$ as prescribed by the empirical expression

$$\frac{d\tilde{\sigma}_o}{d\varepsilon} = \theta_0 \left[1 - \frac{\tanh(2\tilde{\sigma}_o/\tilde{\sigma}_o)}{\tanh(2)}\right],$$

(5)

where $\tilde{\sigma}_o$ is given in terms of the true strain rate $\dot{\varepsilon}$ by

$$\tilde{\sigma}_o = \tilde{\sigma}_o(\dot{\varepsilon})^{1/n}.$$ 

(6)

Here $n = \mu(T) b^2 A / kT$, $b$ is the Burgers vector, and $A$ is an associated energy. Equations (2) and (3)–(6), together with a specified form for the function $f$ in Eq. (3), constitute the mathematical realization of the simple concept of Fig. 1. Parameter values are given in Ref. 4.

Results and Comparison with Experimental Data

Ingots of unalloyed tantalum were forged, rolled, and annealed to yield material with a uniform grain size of 35–38 μm. Some of this material was then shocked to 45 GPa for 1.8 μs using an explosive fixture. Cylindrical specimens 0.5 cm in diameter by 0.5 cm high were prepared from both shocked and unshocked materials and tested on a conventional hydraulic test machine and on a compressive split Hopkinson pressure bar (SHPB).

Calculations at 298 K with constant $\tilde{\sigma}_p$ and $\tilde{\sigma}_p^2$, shown with corresponding experimental data in Fig. 2, reproduce the initial yield stresses very well. At large strains, the agreement remains reasonably good because obstacle hardening is the dominant mechanism. At smaller strains, however, where the Peierls mechanism dominates, plateaus of constant flow stress much wider than those observed become a prominent feature of the calculated flow curves.

To address this discrepancy, we allowed the threshold stress $\tilde{\sigma}_p^2$ in Eq. (3) to increase with deformation according to the relation (Ref. 4)

$$\frac{d\tilde{\sigma}_p^2}{d\varepsilon} = \theta_{p2} \left[1 - \frac{\tilde{\sigma}_p^2}{\tilde{\sigma}_{p20}}\right]^{0.70},$$

(7)

This expression has no physical significance of which we are aware; we selected it because it has a form consistent with data at 77 K (4).

Flow curves recalculated with this modification are compared with the experimental data in Figs. 3 and 4. At 298 K (Fig. 3), the improvement in the agreement at intermediate strains ($\dot{\varepsilon} = 0.1$ and 0.001 s$^{-1}$) is striking (cf. Fig. 2). The description of the SHPB results (Fig. 4) is similarly much improved (4), with modest workhardening controlled by Eq. (7) now a prominent feature. Some hardening of the flow stress at 77 K is also apparent, but here the agreement is not completely satisfactory, presumably because Eq. (7) does not completely capture the changes in $\tilde{\sigma}_p^2$ with deformation. As expected, the introduction of Eq. (7) has no effect on the flow curve at 400 K and an engineering strain rate of 1.6 $\times$ 10$^{-5}$ s$^{-1}$ (Fig. 4) because the obstacle term dominates all but a very limited initial flow regime under these conditions.

* The factor $M(T) = \mu(T)/\mu(28^\circ C)$ in Eq. (3) normalizes the stresses to the temperature-dependent shear modulus.

* Cabot Corporation, Boyertown, Pennsylvania, USA.
Comparison of model calculations of unshocked tantalum for constant $\dot{\varepsilon}_p$ and variable $\dot{\varepsilon}_g$ [Eq. (7)] with experimental observations for various engineering strain rates at 298 K. Calculations assume that deformation takes place isothermally.

After shock loading to 45 GPa, flow behavior is quite different from that of unshocked material. Figure 5 shows flow curves from quasistatic and SHPB experiments with shocked and unshocked materials. The slopes of the curves (the workhardening) at both low and high strain rates are decreased by shock loading, and the initial slope for the quasistatically tested shocked material is considerably less than that of unshocked samples.

It is interesting to note that quasistatic flow curves appear to become parallel at strain above about 0.3. This is unlike the behavior observed in copper (7, 8), in which the flow curves of unshocked material appear to asymptotically approach those of corresponding shocked material, and it suggests that shock loading in unalloyed tantalum changes the athermal component $\sigma_a$ of the flow stress. From the difference between the quasistatic flow curves at $\varepsilon = 0.34$, we estimate that the increase in $\sigma_a$ is 90–100 MPa. For unshocked material we have $\sigma_a = 55$ MPa (4), so we calculate that $\sigma_a = 145$ MPa for our shocked material. Using this value and assuming that the flow stress at the lowest strain rate ($1.9 \times 10^{-5} \text{ s}^{-1}$) is entirely controlled by obstacles, we obtain from Eqs. (2) and (4) a value for the initial obstacle threshold stress of shocked material of $\sigma_o = 283$ MPa.

The appropriate value for the initial threshold stress $\sigma_o$ of the secondary Peierls mechanism for shocked material is difficult to determine directly, but a value of 750 MPa reproduces the flow curves of the shocked material reasonably well. Figure 6 shows flow curves calculated with these values of $\sigma_o$, $\sigma_w$, and $\sigma_g$, but with all other model parameters unchanged from those given in Ref. 4, along with the measured flow curves.

Figure 5. Flow curves at engineering strain rates $\dot{\varepsilon}$ of 4560 and $1.6-1.9 \times 10^{-5} \text{ s}^{-1}$ for shocked and unshocked tantalum.

Figure 6. Measured and calculated flow curves for tantalum after shock loading to 45 GPa for 1.8 $\mu$s.
Discussion

The calculations shown in Fig. 6 agree well with the measured flow curves of shock-loaded material over a wide range of strain rates. It is noteworthy that the pronounced flattening of the flow curves of shocked tantalum relative to the curves of unshocked material is captured well by the hardening of $\dot{\sigma}_t$ and $\dot{\sigma}_2$. The agreement with the SHPB data ($\dot{\varepsilon} = 4560 \text{s}^{-1}$) is also good, and the calculations, which are dominated in this regime by changes in $\dot{\sigma}_{2d}$, successfully reproduce the decrease in the flow stress for strains larger than about 0.1. The principal Peierls energy and stress are apparently unchanged by the shock loading, as we expect if they truly represent an intrinsic Peierls barrier. Similarly, the hardening characteristics of $\dot{\sigma}_t$ and $\dot{\sigma}_{2d}$, which describe the evolution of the underlying structure, remain unchanged from those of unshocked specimens.

Changes in the obstacle threshold stress $\dot{\sigma}_0$ of copper upon shock loading are well documented (7-9), and a similar change in tantalum is not unexpected. Briend and Batchelor (10) report a well-defined polygonal cell structure in shock-loaded tantalum that is absent in unshocked material and that may contribute to the observed increase in $\dot{\sigma}_t$. The 283-MPa increase that we suggest is reasonable, although it is somewhat lower than might be inferred from the data for copper, which shows an increase of 200–250 MPa after being subjected to a 10–12 GPa, 1-µs shock (7, 8).

It is not clear what causes the 90–100 MPa increase (suggested by the data in Fig. 5) in the athermal stress $\dot{\sigma}_s$ following shock loading. Copper does not show a similar effect, at least for shock pressures up to 12 GPa (7, 8), so its behavior cannot be used as a guide. The athermal stress is usually associated with long-range obstacles for which thermal activation plays no role, such as grain boundaries. Consistent with this notion, the athermal stress of copper increases as the grain size decreases (6). While shock loading by itself does not change the grain size, it may nevertheless introduce microstructural features that produce a similar effect. Deformation twin boundaries are one such feature, and have been reported in tantalum deformed at very high rates or very low temperatures (11). Preliminary microstructural observations (10) of the shock-loaded materials studied here do not conclusively reveal deformation twins, but they do show the presence of lens-shaped regions of high dislocation density whose exact nature is as yet unknown. Such features may be related to the increase in the athermal stress suggested by the data in Fig. 5.

The increase in the threshold stress $\dot{\sigma}_{2d}$ of the secondary Peierls term [Eqs. (3) and (7)] is problematic. As for unshocked tantalum, this term appears to be essential to modeling the flow behavior of shocked material properly, particularly at high strain rates (or low temperatures), but it is of special importance at low and intermediate strain rates because it determines the change in initial flow stress with strain rate and accounts for the initial flatness of the flow curves. The physical origin of the secondary term is unknown, however. The increase of $\dot{\sigma}_{2d}$ from 56 to 750 MPa seems rather large, but without a better idea of the underlying mechanism it is impossible to say whether such an increase is reasonable.

Conclusions

From this work we conclude the following:

1. A model based on multiple deformation mechanisms combined in a physically reasonable way can adequately describe the characteristics of plastic flow curves of unalloyed tantalum that has been previously shock loaded.

2. Within such a model, only three structural parameters (the athermal stress $\dot{\sigma}_t$ and the threshold stresses $\dot{\sigma}_0$ and $\dot{\sigma}_{2d}$ for obstacles and the secondary Peierls barrier, respectively) must be changed from those of unshocked material to reproduce the observed flow curves of shocked material over a wide range of strain rates.

3. Model parameters and characteristics other than the structural parameters are the same for both shocked and unshocked materials. In particular, the principal Peierls barrier $G^p$, and the workhardening characteristics are unchanged by shock loading.

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