PPM Newsnote

Density Functional Theory (DFT) provides ab-initio, electronic structure based predictions of elastic-plastic constants in Ta, W, and Ta-W alloys

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Mesoscale models of metal deformation rely on parameters that describe their elastic properties and dislocation plasticity. As part of the Predicting Performance Margins (PPM), simulation data from our recent DFT calculations have been used to parameterize a crystal plasticity model for Ta-W alloys of arbitrary composition, in a way that captures not only the dislocation plasticity, but also the temperature and strain rate dependence thereof.

Table 1 shows basic material properties (lattice parameter and elastic constants) and parameters that describe dislocation "lattice friction" for pure Ta, pure W, and the 50/50 alloy of TaW. The lattice friction parameters are needed for our novel model of temperature and rate-dependent yield of BCC metals, described by

$$\tau^*_{\mathrm{EI}} = \tau_0^{\mathrm{EI}} \left(1 - \frac{T}{T_{\mathrm{c}}}\right)^2 = \tau_0^{\mathrm{EI}} \left(1 - \frac{k_{\mathrm{B}} T \ln(\dot{\gamma}_0/\dot{\gamma})}{2H_k}\right)^2 \tag{1}$$

$$\tau^*_{\mathrm{LT}} = \tau_0^{\mathrm{LT}} \left(1 - \left(\frac{T}{T_{\mathrm{c}}}\right)^{1/2}\right) = \tau_0^{\mathrm{LT}} \left(1 - \sqrt{\frac{k_{\mathrm{B}} T \ln(\dot{\gamma}_0/\dot{\gamma})}{2H_k}}\right) \tag{2}$$

where EI is the Elastic Interaction regime where dislocation kink pairs are well-formed and the dislocation line between them rests in the adjacent Peierls valley, and LT is the Line Tension regime where kinks are not well formed such that the dislocation line bows out and does not reach the adjacent Peierls valley. Figure 1 shows plots of elastic constants (needed for the elastic portion of our crystal-elastic-plastic constitutive capability), and yield stresses (obtained by implementing Equations 1 and 2 into our crystal plasticity finite element simulations) validated against experimental data.

This capability will enable the quantification of microstructure-induced variability in the performance of Ta-W alloy components in both normal and abnormal thermal and mechanical environments. The PPM program is jointly funded by ASC P&EM, RTBF, and ESC.

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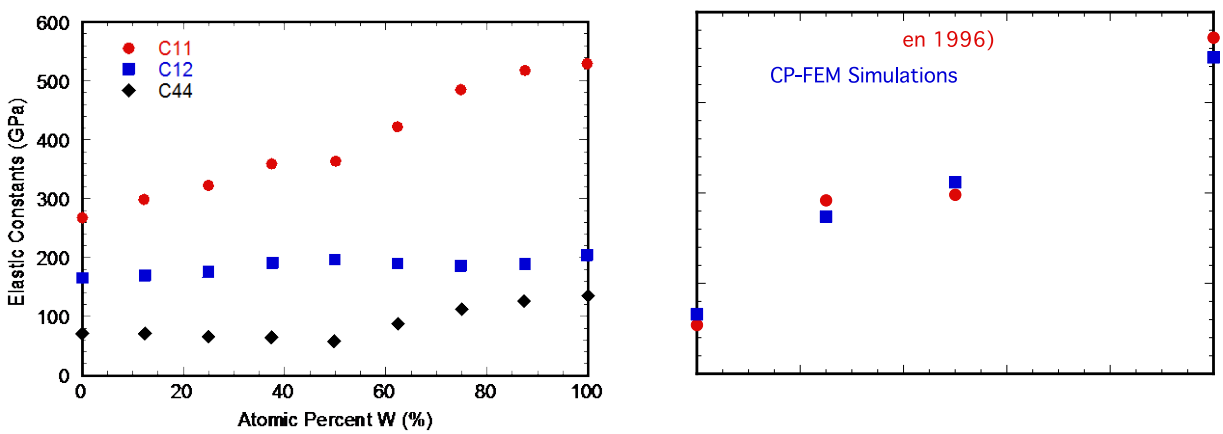
Table 1. Material properties, and temperature and rate-dependent lattice friction parameters, for Ta, W, and TaW.

	Ta	W	TaW
a (Å)	3.30	3.16	3.23
C_{11} (GPa)	265	523	369.5
C_{12} (GPa)	160	203	182.5
C_{44} (GPa)	82.3	160	88
$2H_k$ (eV)	0.85	2.06	1.20
τ_0^{EI} (MPa)	406	2035	1031
τ_0^{LT} (MPa)	320	1038	679
$\ln\dot{\gamma}_0$	15	24	19.5



(a) (b)

Figure 1. Material constants for Ta-W alloys as functions of composition, showing (a) elastic constants and (b) yield stress (i. e. slip resistance) validated by experimental data.

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