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EoS

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Starck Ta PTW strength model recommendation for use with Sesame 93524 EoS

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1 Introduction

The purpose of this document is to provide a calibration of the Preston-Tonks-Wallace (PTW) [1] strength model for use with the Sesame equation of state (EoS) 93524 [2]. The calibration data included in this fit spans temperatures from 198 K to 673 K and strain rates from 0.001/s to 3200/s.

2 Shear modulus - thermal model

The linear Preston-Wallace [3] model of the shear model has been fit to a polycrystalline Voight shear modulus average as described in the previous document [4], but this time the density correction has been performed using the isothermal bulk modulus, thermal expansion and solidus melt curve from the SESAME EoS 93524 tables. The result is that the thermoelastic shear modulus parameter has been changed from $\alpha = 0.45$ to $\alpha = 0.21$. The fit is described by

$$G(\rho, T) = G(\rho) \left(1 - \alpha \frac{T}{T_m(\rho)} \right), \quad (1)$$

with $G_0 = G(\rho = 16.753) = 0.699$ Mbar and $\alpha = 0.21$. This fit is shown in Figure 1. This factor of G_0 is only used for the fit. This thermoelastic coefficient α , here determined empirically from data, agrees with the thermoelastic behavior found using quantum molecular dynamics (QMD) simulations. Due to a lack of data at arbitrary pressures and densities, the QMD data is used to specify the cold shear modulus as a function of density.

3 Parameter fit

The calibration data used to fit the PTW model are listed in Table 1. These data were kindly provided by the MST-8 group at Los Alamos [5]. The dynamic data sets were weighted such that any three dynamic data sets at a given temperature and strain rate had the same weight as one of the quasistatic data sets, which

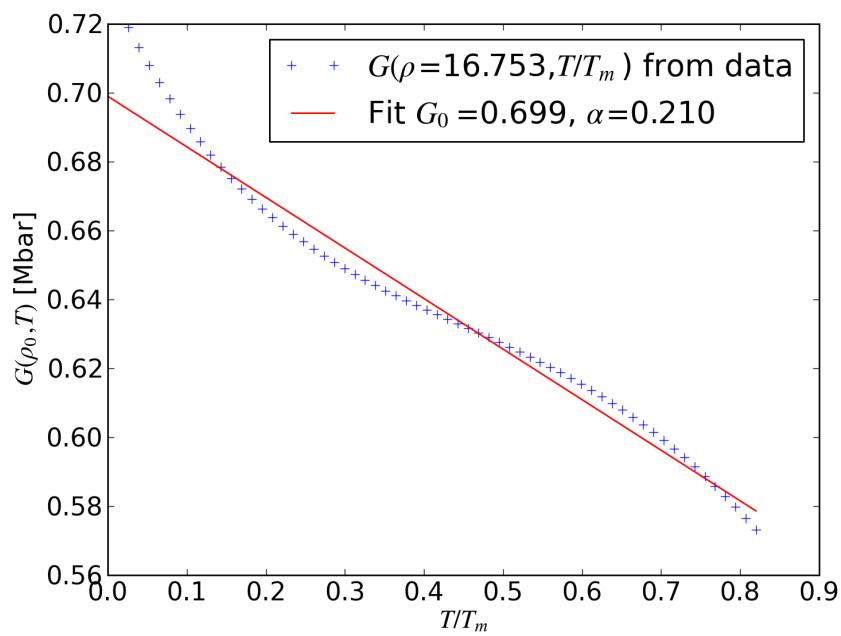


Figure 1: Fit to shear modulus data

Strain rate [1/s]	ψ_{min}	ψ_{max}	T [K]	Adiabatic?	C_V [J/kg/K]	Q/W
1600.0	0.02	0.09	473.0	yes	140.6	1.0
1700.0	0.12	0.19	473.0	yes	140.6	1.0
1800.0	0.22	0.29	473.0	yes	140.6	1.0
1900.0	0.016	0.109	673.0	yes	143.4	1.0
1800.0	0.16	0.23	673.0	yes	143.4	1.0
2100.0	0.275	0.36	673.0	yes	143.4	1.0
0.001	0.02	1.08	293.0	no	-	-
0.001	0.006	0.2	293.0	no	-	-
2400.0	0.024	0.076	293.0	yes	136.0	1.0
2800.0	0.105	0.168	293.0	yes	136.0	1.0
3200.0	0.2	0.27	293.0	yes	136.0	1.0
0.1	0.014	1.0	373.0	no	-	-
0.1	0.004	1.0	473.0	no	-	-
0.1	0.035	1.0	248.0	no	-	-
1200.0	0.012	0.064	198.0	yes	132.9	1.0
1200.0	0.078	0.135	198.0	yes	132.9	1.0
1300.0	0.15	0.2	198.0	yes	132.9	1.0

Table 1: Calibration data

include a much larger range of strains. The one exception is the seventh entry in the table, which was given twice as much weight because of the large range of strain covered.

Between the initial fit to the Grüneisen EoS and the first pass at a fit to these calibration data with the new SESAME EoS, we found that the Grüneisen fit was too weak at Taylor rod strain rates on the order of 10^5 /s, while the initial SESAME fit was too strong. The dominant contributing factor was found to be the rate-dependent constant γ . Values of $\gamma < 10^{-6}$ were found to provide the best fit over the strain rates of the calibration data, with residual errors of less than 5%. However, these values of γ dramatically increase the strength at strain rates of a few 10^5 /s. The fit as given uses a value of γ fixed such that the average error found with respect to the calibration data is $< 10\%$.

The specific heat used for adiabatic treatment during fitting was a simple polynomial form which matches the EoS over a sufficient temperature range, $C_V = 124.641 + 0.0476576T - 2.92585 \times 10^{-5}T^2$ J/kg/K.

4 Summary

The residual weighted error is 9.3% for the 17 data sets fit to obtain this parameter set. Figure 3 shows a comparison between this fit and the calibration data. The recommended fit parameters are given in Table 2. A sample FLAG [6] input deck is given in the following section and Figure 3 shows a comparison

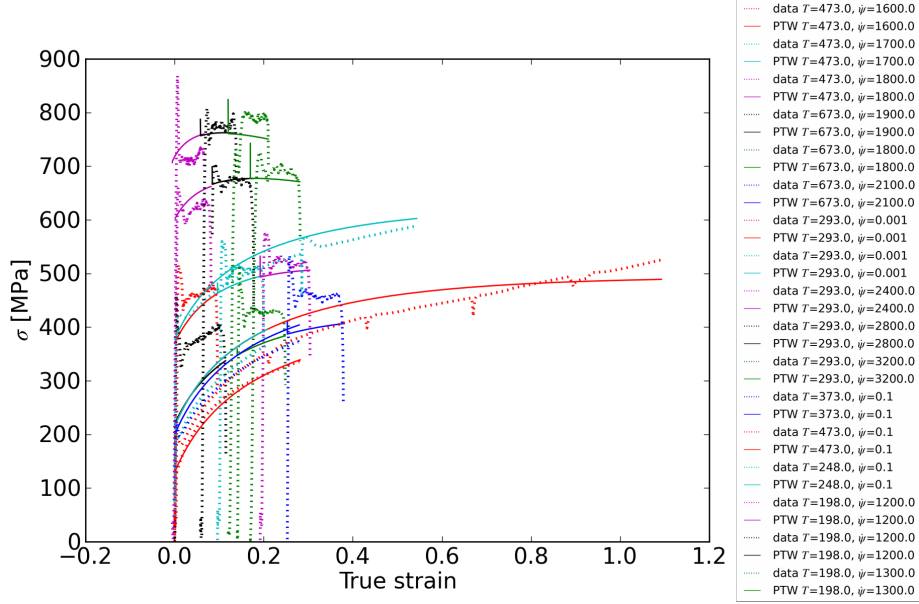


Figure 2: Strength model fit compared with all included calibration data

between FLAG outputs and the calibration curves.

5 Supplementary information

To facilitate direct use of the generalized BGP model for the shear modulus instead of the Sesame table, we specify its parameters for Ta. In the notation of Equation 5 of [7], the model for the shear modulus is

$$G(\rho_{ref}, 0) = 72.2 \text{ GPa}, \quad \rho_{ref} = 16.74 \text{ g/cc}, \quad (2)$$

$$\gamma_1 = 3.0567, \quad \gamma_2 = -6.6, \quad (3)$$

$$q_1 = 1/3, \quad q_2 = 1.0. \quad (4)$$

In a form more amenable to unit conversion, we instead write

$$G_0(\rho, T = 0) = G_{ref} \left(\frac{\rho}{\rho_0} \right)^{4/3} \exp[X(\rho)], \quad (5)$$

$$X(\rho) = \sum_{k=1}^N \frac{2a_k}{q_k} \left[\left(\frac{b_k}{\rho_{ref}} \right)^{q_k} - \left(\frac{b_k}{\rho} \right)^{q_k} \right], \quad (6)$$

with $a_k = \text{sign}(\gamma_k)$ and $b_k = |\gamma_k|^{1/q_k}$. In this formulation, the coefficients a_k are dimensionless and the coefficients b_k have the same units as the density, ρ .

Parameter	Final value
θ	0.0142
p	5.000
s_0	0.008128
s_∞	0.002772
κ	0.5525
γ	8×10^{-6}
y_0	0.007275
y_∞	0.000604
y_1	0.012700
y_2	0.400000
β	0.23
G_0 [Mbar]	0.699
M_A [g/mol]	180.94788
M_A [g/atom]	3.0047×10^{-22}
α	0.21

Table 2: PTW fit parameters for Starck Ta with SESAME EoS 93524

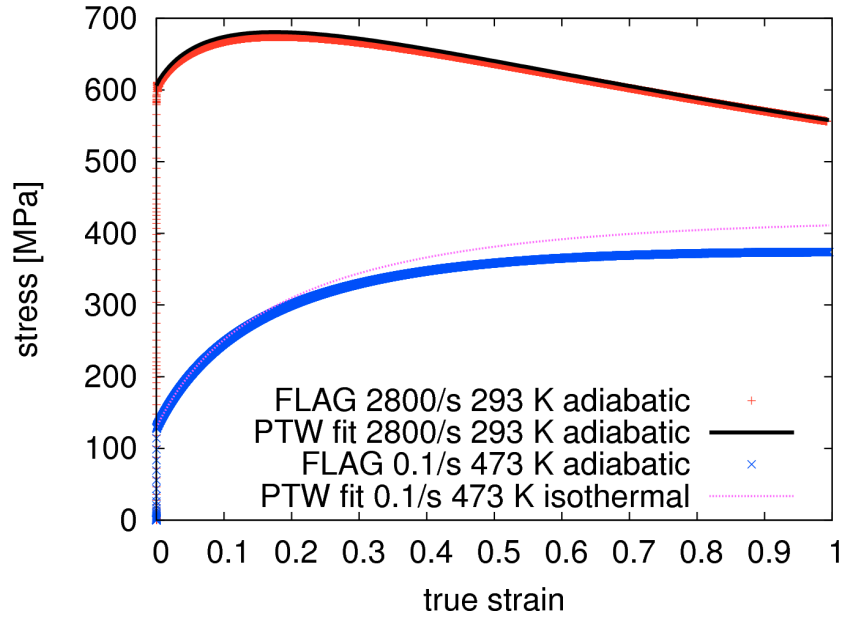


Figure 3: Comparison between FLAG output and corresponding calibration curves. The discrepancy between the quasistatic curve at larger strains and the calibration curve is due to the fact that it was simulated adiabatically in FLAG.

With this representation, the cold shear modulus is specified by

$$G(\rho_{ref}, 0) = 72.2 \text{ GPa}, \quad \rho_{ref} = 16.74 \text{ g/cc}, \quad (7)$$

$$a_1 = 1, \quad a_2 = -1, \quad (8)$$

$$b_1 = 28.56, \quad b_2 = 6.6, \quad (9)$$

$$q_1 = 1/3, \quad q_2 = 1.0. \quad (10)$$

References

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- [2] SESAME 93524, Carl Greeff, for Los Alamos Advanced Simulation and Computing, Physics and Engineering Models program, Equation of State project (2017)
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- [7] Leonid Burakovsky, D.J. Luscher, Dean Preston, Sky Sjue and Diane Vaughan, *Generalization of the Unified Analytic Melt-Shear Model to Multi-Phase Materials: Molybdenum as an Example* **2019**, 9, 86.