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Half-hard copper PTW model parameters for plastic deformation calibrated to strain rates from 10^{-3}–10^{7}/s

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This document demonstrates a calibration of the Preston-Tonks-Wallace (PTW) model of plastic deformation [1] that fairly accurately reproduces the flow stress of half-hard copper across strain rates varying by a factor of more than ten billion. The experiments included are quasistatic compression at low rates, Split Hopkinson Pressure Bar (SHPB) compression [2] at intermediate rates, and arrested Richtmyer-Meshkov instability (RMI) growth [3, 4] at high strain rates. The temperatures vary from liquid nitrogen (77 K) to around 500 K. The largest true strains obtained are approximately 0.5. It would be interesting to compare the results to copper deformation data at higher pressures and higher strains.

1 Shear modulus parameters for Preston-Wallace model

We use the shear modulus model of Preston and Wallace [5]. The shear modulus is taken to be a function of density and temperature,

$$G(\rho, T) = G_0(\rho)\left(1 - \alpha\frac{T}{T_m(\rho)}\right), \tag{1}$$

where $G_0(\rho)$ is the shear modulus as a function of density at $T = 0$ and $T_m(\rho)$ is the melt temperature (solidus) as a function of density. We have used the Sesame table 33330 for the cold shear modulus and Sesame table 3337 [6] for all equation of state quantities.

We determined the value of α from experimental data in a fashion consistent with the 3337 Cu EoS. First we obtained ambient pressure Cu shear modulus data from Simmons and Wang [7]. Then we corrected this data to constant density using the Preston and Wallace formula

$$G(\rho_0, T) = G(\rho, T) + \left(\frac{\rho_0}{\rho} - 1\right) B_T(\rho, T)\left(\frac{\partial G}{\partial P}\right)_{T,P=0}. \tag{2}$$

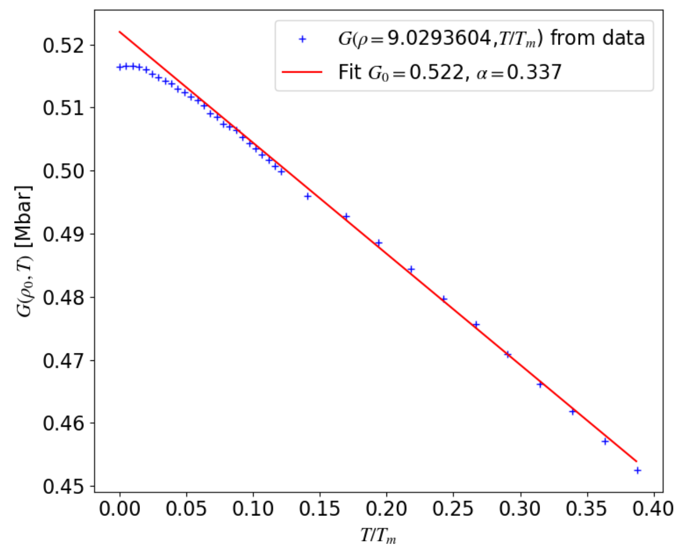

Figure 1: Determination of the thermoelastic parameter α from a combination of ambient shear modulus data and equation of state information. The blue '+' symbols are the corrected data points and the red curve is the linear fit. Depending on whether the minimum value of the homologous temperature T/T_m used in the fit was 0.1 or 0.15, values were found slightly larger or smaller than $\alpha = 0.34$. A value with two significant figures was chosen for simplicity.

In this equation, $G(\rho, T)$ is the ambient data, $\rho(P = 0, T)$ and $B_T(\rho, T)$ come directly from the 3337 Cu EoS, and $\partial G/\partial P$ is found by taking $\partial G/\partial \rho$ from the cold shear table 33330 and multiplying it by $\partial \rho/\partial P$ from the 3337 Cu EoS. The actual value used was $\partial G/\partial P$=1.5. The thermoelastic parameter was found to be $\alpha = 0.34$. A fit resulting in a value close to this is shown if Figure 1.

2 Calibration method

The data sets used in the model calibration are shown in Table 1. The quasistatic data are treated as isothermal, but the SHPB data are treated adiabatically. The arrested RMI data sets are treated as if they were ambient. In reality there is an initial shock followed by a release, so the temperature and pressure are modified, but the effect is not expected to be large. This assumption has been validated now with FLAG simulations [8] of the RMI experiments with this parameter set[1].

[1]Thanks to Thao Nguyen for running these simulations.

Table 1: Data sets used in the calibration along with the details of their treatment. Q/W is the fraction of plastic work converted into internal energy (heat). Any energy stored by creation of dislocations is neglected.

Strain rate [1/s]	ψ_{min}	ψ_{max}	T [K]	Adiabatic?	C_V [J/kg/K]	Q/W	weight
0.1	0.004	1.0	298.0	no	-	-	1.5632
0.001	0.005	1.0	298.0	no	-	-	1.7717
2000.0	0.0	0.18	298.0	yes	384.2	1.0	0.6567
2800.0	0.22	1.0	298.0	yes	384.2	1.0	0.4305
2000.0	0.02	1.0	473.0	yes	405.8	1.0	0.4439
0.001	0.0	1.0	77.0	no	-	-	1.5157
6000000.0	0.0	1.0	298.0	no	-	-	39.8625
40000000.0	0.0	1.0	298.0	no	-	-	79.7250

A match was obtained to the arrested RMI data first as follows. The high rate limit of the PTW model is

$$\sigma = 2Gs_0(\dot{\varepsilon}/\gamma\dot{\xi})^{\beta}. \quad (3)$$

The characteristic strain rate $\dot{\xi} \approx 8 \times 10^{12}$/s for copper. Based on the RMI data sets, it is implied that $\beta \approx 0.44$. This can be compared with the value 0.25 given in the original PTW paper, which was based on a theoretical model above 10^8/s along with inclined flyer gas gun data at rates from 10^5–10^7/s [9]. The uncertainties in the arrested RMI data sets would admit slightly larger or smaller values of β, but the original value of 0.25 seems inconsistent. These earlier data feature significantly smaller strains than the arrested RMI data, so only the latter are used in this calibration. Given this value of β, the parameters s_0 and γ are strongly correlated, so effectively only one remains free to calibrate the rest of the data. Based on the given value here of $\gamma = 5 \times 10^{-7}$, the transition from the thermal activation regime to the overdriven shock limit occurs at $\dot{\varepsilon} \approx 4 \times 10^6$/s.

The parameters y_1 and y_2 were constrained to be equal to s_0 and β, respectively. This practice has previously been used for SHPB data [10], with the intention to potentially further modify y_1 and y_2 in the parameter set for a better match to flyer plate shock data at small strains.

The quasistatic and SHPB were used to fit s_0, s_∞, y_0, y_∞ and κ with γ fixed. There was very little sensitivity so the value $p = 1$ was fixed. The initial values of s_0 and γ were chosen to match the arrested RMI data. As the value of s_0 was modified to fit the quasistatic and SHPB data, it was necessary to modify γ to remain consistent with the arrested RMI data. The final combination matches all of the data acceptably well. If one were to ignore the arrested RMI data, it would be possible to match the other data sets with RMS variation around 2% with a significantly larger (perhaps unphysical) value of s_0. Agreement with the arrested RMI data limits the magnitude of s_0.

3 Summary

The RMS difference between the data and the model is 7.4%, given by

$$RMS = \sqrt{\Delta^2/N}, \tag{4}$$

$$\Delta^2 = \sum_{j=1}^{8}\sum_{i=1}^{n_j} w_j (d_{ji} - f_{ji})^2/d_{ji}^2, \tag{5}$$

$$N = \sum_{j=1}^{8}\sum_{i=1}^{n_j} 1, \tag{6}$$

$$w_j = (N/8)/n_j. \tag{7}$$

In this scheme, n_j is the number of data points in data set j and w_j ensures equal weight for each data set. The recurring value of 8 is the total number of data sets used in this calibration: three quasistatic experiments, three split Hopkinson pressure bar experiments, plus two arrested RMI experiments. d_{ji} is the i^{th} value from data set j and f_{ji} is the corresponding flow stress value from the PTW strength model. A comparison between this strength model and the data sets is shown in Figure 2.

Parameter	Value
θ	0.0283
p	1.0
s_0	0.0047
s_∞	0.002
κ	0.1191
γ	5.0e-7
y_0	0.0024
y_∞	0.0012
y_1	0.0047
y_2	0.44
β	0.44
G_0 [Mbar]	0.519
M_A [g/mol]	63.546
α	0.34
$T_m(\rho_0)$	2064.0
ρ_0	9.03

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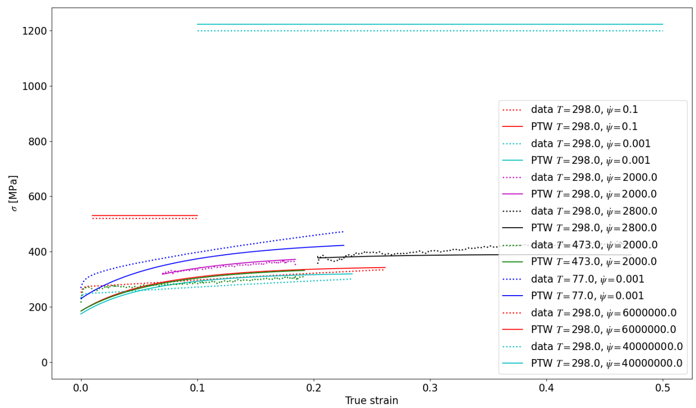

Figure 2: Dots show the data sets while the continuous lines show the PTW model. The two highest flow stress "data sets" are adapted from the arrested RMI experiments. They are based on estimates of the flow stress made by Michael Prime using FLAG simulations.

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