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**Title:** The Proportion of Plastic Work Converted to Heat in T16AL4V:  
MTS Model Prediction and Experimental Data

**Author(s):** Duncan A.S. Macdougall, MST-8  
Paul J. Maudlin, T-3

**Submitted to:** Explomet 2000  
June 19-23, 2000  
Albuquerque, NM

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# The proportion of plastic work converted to heat in Ti-6Al-4V: MTS model prediction and experimental data

Duncan A. S. Macdougall<sup>1</sup> and Paul J. Maudlin<sup>2</sup>

<sup>1</sup>MST-08: Structure Property Relationships, MS: G755

<sup>2</sup>T-03: Fluid Dynamics, MS: B216

Los Alamos National Laboratory, Los Alamos, NM 87545, USA.

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## 1. ABSTRACT

The thermodynamics-based Mechanical Threshold Stress (MTS) model, proposed by Mecking and Kocks [1] and implemented by Follansbee and Kocks [2], has been used to make predictions of the proportion of plastic work converted to heat,  $\beta$ , in the alloy Ti-6Al-4V. This alloy is widely used in the aerospace industry to manufacture components that are designed to resist impact, such as fan-blades. Accurate knowledge of  $\beta$  and its variation with plastic strain are necessary to produce reliable finite element simulations involving high strain-rate plastic deformation.

The necessary material constants for the MTS model were found by Follansbee and Gray [3] from compression experiments on Ti-6Al-4V over a range of temperatures and strain rates. High strain-rate torsion tests were performed on Ti-6Al-4V using a torsional split-Hopkinson pressure bar at a strain rate of  $400\text{s}^{-1}$  [4]. An infrared radiometer [5] was used to follow the surface temperature of the specimen during the test. The experimental measurement of  $\beta$  is compared to the MTS model prediction. Both results indicate that  $\beta$  is initially a strong function of strain, and saturates at higher plastic strains.

## 2. INTRODUCTION

The conversion rate of plastic work to heat,  $\beta$ , is an important quantity. It is necessary in finite element simulations involving plasticity in which temperature calculations are made. Accurate knowledge of  $\beta$  is especially important in FE simulations of impact events in which adiabatic

heating may occur, resulting in large temperature rises.

Considerable efforts are being made in this field both to measure  $\beta$  experimentally [4, 6-11] and to describe the evolution of  $\beta$  analytically [12, 13]. Although a number of researchers have found values of  $\beta$  which vary with plastic strain and may be lower than the classical assumption of 0.9-0.95, these results remain controversial and have split the scientific community.

In this work, the MTS model, with constants derived previously [3], is compared to experimental measurements of the variation of  $\beta$  with plastic strain for Ti-6Al-4V. The experiment was performed in high-speed torsion with the surface temperature measured using radiometry. Two modifications are made to the MTS model to account for differences between the initial state of the material used to derive the model and that used to conduct the experiments.

## 3. MTS MODEL FOR Ti-6Al-4V

### 3.1 MTS model formulation for $\beta$ predictions

Consider a specific internal energy function that depends on the *displacement* variables of elastic strain (tensor), entropy and stored dislocation density:

$$U = U(\underline{\underline{\epsilon}}^e, S, \rho_d)$$

where a normalized density is used here that involves the saturation density of stored dislocations:

$$\rho_d \equiv \bar{\rho}_d / \bar{\rho}_s$$

and  $\underline{\underline{\epsilon}}$  is a total strain measure. Now, for an

adiabatic process and no external heat source:

$$\dot{U} = \frac{1}{\rho} \underline{\underline{\sigma}} : \underline{\underline{D}}$$

We next assume that our strain measure and the rate-of-strain can be partitioned into elastic and plastic parts:

$$\underline{\underline{\epsilon}} = \underline{\underline{\epsilon}}' + \underline{\underline{\epsilon}}^p \Rightarrow \underline{\underline{D}} = \underline{\underline{D}}' + \underline{\underline{D}}^p$$

Applying the chain rule to  $\dot{U}$  observant of the dependencies appearing in Eq. (1), we obtain the result:

$$\dot{U} = \frac{\partial U}{\partial \underline{\underline{\epsilon}}} : \underline{\underline{D}} + \frac{\partial U}{\partial \underline{\underline{\epsilon}}^p} : \underline{\underline{D}}^p + \frac{\partial U}{\partial S} \dot{S} + \frac{\partial U}{\partial \rho_d} \dot{\rho}_d$$

We now introduce constitutive relationships that define the thermodynamic forces conjugate to their respective thermodynamic displacements:

$$\underline{\underline{\sigma}} \equiv \rho \frac{\partial U}{\partial \underline{\underline{\epsilon}}} \quad , \quad \underline{\underline{\sigma}}' \equiv \rho \frac{\partial U}{\partial \underline{\underline{\epsilon}}'} \quad , \quad \underline{\underline{\sigma}}^p \equiv -\rho \frac{\partial U}{\partial \underline{\underline{\epsilon}}^p} \quad , \quad T = \frac{\partial U}{\partial S} \quad , \quad \tilde{\sigma} \equiv \rho \frac{\partial U}{\partial \rho_d} \quad (6)$$

Observe in these relationships that positive and negative signs are assigned to distinguish between intrinsic sinks or sources of energy, respectively. Combining Eqs. (3), (5) and (6), we obtain the result:

$$\underline{\underline{\sigma}} : \underline{\underline{D}}^p - \tilde{\sigma} \dot{\rho}_d = \rho T \dot{S}$$

and identify the right-hand-side (RHS) of this equation as  $D_r$  that is subject to the Second Law (Clausius-Duhem in the absence of heat conduction and external heat sources):

$$D_r \equiv \rho T \dot{S} \geq 0$$

Since we are emphasizing plasticity, we assume negligible elastic strain and insert  $T \dot{S} \equiv C_v \dot{T}$  into Eq. (7) and recover a thermal relationship:

$$\rho C_v \dot{T} = \underline{\underline{\sigma}} : \underline{\underline{D}}^p - \tilde{\sigma} \dot{\rho}_d$$

An instantaneous definition for  $\beta$  can now be obtained by integrating Eq. (9) for the temperature rise:

$$\Delta T = \frac{1}{\rho C_v} \int_0^t \left[ \underline{\underline{\sigma}} : \underline{\underline{D}}^p - \tilde{\sigma} \dot{\rho}_d \right] dt' = \frac{1}{\rho C_v} \int_0^t \beta \underline{\underline{\sigma}} : \underline{\underline{D}}^p dt' \quad (10)$$

where

$$\beta \equiv \frac{\underline{\underline{\sigma}} : \underline{\underline{D}}^p - \tilde{\sigma} \dot{\rho}_d}{\underline{\underline{\sigma}} : \underline{\underline{D}}^p} = \frac{D_r}{\underline{\underline{\sigma}} : \underline{\underline{D}}^p} \quad (4)$$

The work term  $\tilde{\sigma} \dot{\rho}_d$  appearing in this definition physically represents an energy sink (when  $\dot{\rho}_d > 0$ , thus the negative sign in Eq. (11)) as intragranular dislocation structures form during plastic deformation, or at high enough temperatures  $\tilde{\sigma} \dot{\rho}_d$  could represent an energy source (when  $\dot{\rho}_d < 0$ ) as dislocation structures are annihilated.

The standard equations for the MTS flow stress are:

$$\sigma = \sigma_a + \frac{\mu}{\rho_d \mu_0} (s_D \hat{\sigma}_D + s_I \hat{\sigma}_I + s_S \hat{\sigma}_S) \quad \tilde{\sigma} \equiv \rho \frac{\partial U}{\partial \rho_d}$$

$$s_{D,I,S} = \left[ 1 - \left( \frac{kT}{g_{0,D,I,S} \mu b^3} \ln \frac{\dot{\epsilon}_{0,D,I,S}}{\epsilon} \right)^{\frac{1}{q_{D,I,S}}} \right]^{\frac{1}{p_{D,I,S}}}$$

Here the mechanical threshold  $\hat{\sigma}$  is evolved with a differential equation that represents a dynamic balance between dislocation storage and recovery processes at zero degrees Kelvin:

$$\frac{\partial \hat{\sigma}_D}{\partial \epsilon^p} = \Theta_0 [1 - F(\hat{\sigma}_D / \hat{\sigma}_{Ds})]$$

Using the relationship between  $\hat{\sigma}_D$  and a scalar measure of the stored dislocation density  $\hat{\rho}_d$ ,

$$\hat{\sigma}_D = \kappa \mu b \sqrt{\hat{\rho}_d} \quad \text{or inversely} \quad \hat{\rho}_d = \left( \frac{\hat{\sigma}_D}{\kappa \mu b} \right)^2 \quad (15)$$

and keeping Eqs. (2) and (14) in mind, it is important to recognize that  $\tilde{\sigma} \dot{\rho}_d$  is storing dislocations at the same strain-rate and temperature state as that associated with the plastic deformation:

$$\tilde{\sigma} = \frac{\mu}{\mu_0} s_D \hat{\sigma}_D$$

and

$$\rho_d = \left( \frac{\dot{\sigma}}{\dot{\sigma}_s} \right)^2 = \left( \frac{\hat{\sigma}}{\hat{\sigma}_s} \right)^2$$

In order to relate the work term  $\dot{\sigma} \rho_d$  to familiar MTS model quantities, the time derivative is taken of Eq. (17). Using the chain rule and substitution into Eq. (13) yields a  $\beta$ -relationship involving only MTS model quantities:

$$\beta = 1 - \frac{2s_D \left( \frac{\hat{\sigma}_D}{\hat{\sigma}_{Ds}} \right)^2 \Theta_o [1 - F(\hat{\sigma}_D/\hat{\sigma}_{Ds})]}{\frac{\mu_o}{\mu} \sigma_a + (s_D \hat{\sigma}_D + s_I \hat{\sigma}_I + s_s \hat{\sigma}_s)} \quad (18)$$

The constants used by Follansbee [3] to describe the Ti-6Al-4V alloy are shown in Table 1.

### 3.2 Alteration of the MTS constant, $\hat{\sigma}_I$ .

In order to make a valid comparison between the MTS model prediction and experimental measurement of  $\beta$  for Ti-6Al-4V, the material conditions must be examined.

The Ti-6Al-4V alloy material (M1) characterised for the MTS model [3] was solution treated (800°C 1hr, water quenched) and age hardened (500°C 8hrs). This material had a grain size of  $\approx 5\mu\text{m}$ . The material used in the dynamic torsion experiments with temperature measurement [4] (M2) was in an as-received condition. It had been hot-rolled and had a grain size of  $\approx 20\mu\text{m}$ . A slight difference was evident in the chemistry of the two materials, though knowledge of the chemistry for M2 was incomplete. Since the model flow stress was found to overestimate the flow stress in the experiment, it was assumed that the difference in chemistry and the resulting difference in interstitial atom content was responsible. To compensate for this, the interstitial atom threshold stress,  $\hat{\sigma}_I$ , was increased to Z MPa. This value was chosen so as to produce the closest agreement between the experimental and MTS model flow stress.

The alteration of  $\hat{\sigma}_I$  to produce a better correlation between experiment and model is

probably mainly due to the differences in chemistry between materials M1 and M2 – most (probably) oxygen content. However, another possibility is the difference in grain size. The larger grain size of M2 would have the effect of reducing the athermal stress. Also, the MTS model for Ti-6Al-4V was developed using compression tests whereas the experiment used for comparison here was performed in torsion. This is likely to produce differences in texture development. Since the cause for the discrepancy is unknown and likely to be a combination of the above effects, an assumption was made that value of  $\hat{\sigma}_I$  was solely responsible.

### 3.3 Modifications to the MTS model to include prior cold work

Since material M2 used in the experiments contained a considerable amount of prior cold work, unlike M1, an adjustment to the form of the model was necessary.

The evolution of strain hardening in the MTS model is described in Eq. (14). To derive an expression for  $\hat{\sigma}_D$ , this equation is integrated with respect to plastic strain. For an annealed material, the initial stress due to dislocation interactions is zero, so the lower limit of integration for  $\hat{\sigma}_D$  is zero. By making this lower limit non-zero, an initial stress due to dislocation-dislocation interactions – or cold work – can be included. This process yields the following equation:

$$\hat{\sigma}_D = \hat{\sigma}_{Ds} \left[ 1 - \left( 1 - \frac{\hat{\sigma}_{D0}}{\hat{\sigma}_{Ds}} \right) e^{-\Theta_o \frac{\epsilon_p}{\hat{\sigma}_{Ds}}} \right] \quad (19)$$

where  $\hat{\sigma}_{D0}$  is the initial dislocation-dislocation interaction stress caused by prior cold work.

The prior cold work in the Ti-6Al-4V plate used for the  $\beta$  experiments was probably between 10% and 40% plastic strain. This corresponds to an initial dislocation-dislocation interaction stress,  $\hat{\sigma}_{D0}$ , of between X MPa and Y MPa.

Table 1  
MTS model constants for Ti-6Al-4V [3].

Type of obstacle:	p	q	$G_0$	$\dot{\epsilon}_0$	$\hat{\sigma}$
Forrest dislocations, D	2/3	1	1.6	$1.0 \times 10^{10} \text{ s}^{-1}$	See Eq.(15)
Interstitial atoms, I	1	2	0.264	$1.0 \times 10^{10} \text{ s}^{-1}$	1050 MPa
Solute atoms, S	1	2	0.8	$5.8 \times 10^6 \text{ s}^{-1}$	873 MPa
Other constants:					
$\hat{\sigma}_{D_0} = 538 \text{ MPa}$ $\Theta_0 = 2721 \text{ MPa}$ $b = 0.296 \text{ nm}$ $\kappa = 2$ $F = 1$					

#### 4. RESULTS

The MTS model predictions of flow stress are compared to the torsion experiment in Figure 1. These curves were derived using the constants shown in

Table 1, but with two changes detailed in the previous sections.

The MTS curves are shown for several values of the initial dislocation-dislocation interaction stress,  $\hat{\sigma}_{D_0}$ . These curves correspond to an initial cold work of 10%, 20%, 30% and 40%. As the prior cold work increases, the yield stress increases and the subsequent slope decreases, as

expected. Comparing the slope of the MTS model curves to the experimental curve, best agreement is found between 20% and 30% initial cold work.

The proportion of plastic work converted to heat,  $\beta$ , as measured experimentally and predicted by the MTS model is shown in Figure 2. Error bars are shown on the experimental curve. The horizontal error bars correspond to the uncertainty in the measurement of specimen gauge length of  $\approx 3\%$ . The vertical error bars relate to the uncertainty in temperature measurement, which is a combination of the errors in calibration and analysis. The errors are larger at lower temperatures where the radiometer is less efficient.

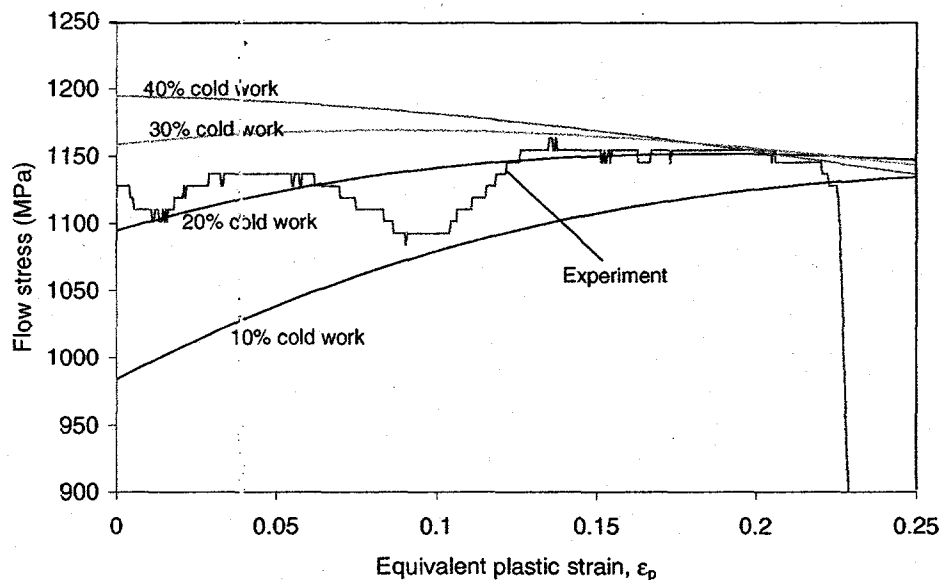


Figure 1 Flow stress: Experiment and MTS model prediction for several values of cold work.



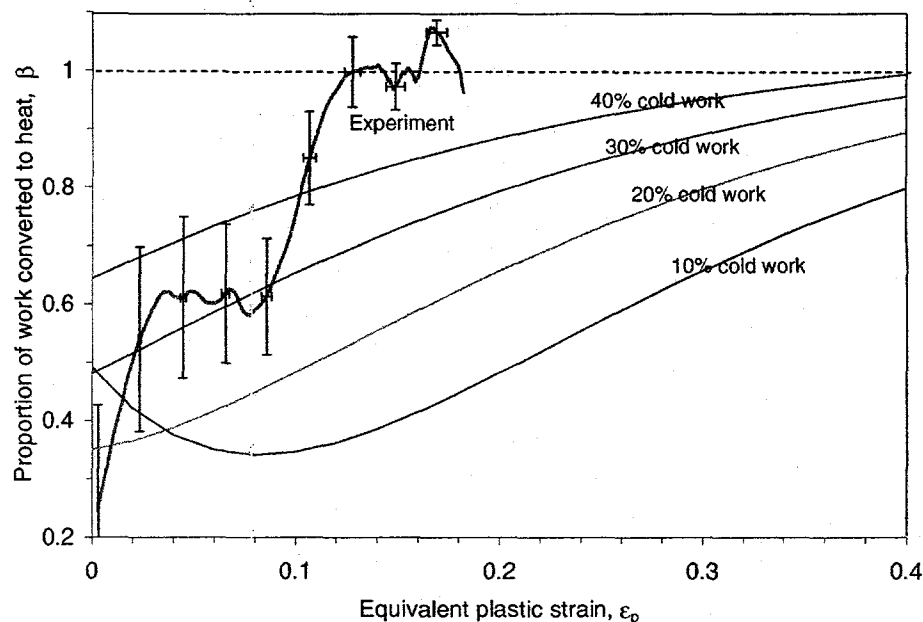


Figure 2 Conversion rate of plastic work into heat for Ti-6Al-4V: Experiment and MTS model predictions for several values of cold work.

The general variation of  $\beta$  with plastic strain measured experimentally is captured well by the MTS model predictions. Both the experiment and model show an increase in  $\beta$  with plastic strain. The best agreement is found using 30% cold work, a similar quantity to that which gave best agreement in the flow stress.

Whilst the general shape of the experimental curve is captured, the detail is not. The experimental curve saturates to  $\beta=1$  much earlier than the model, suggesting that the rate of strain hardening may be higher than the model predicts.

## 5. CONCLUSIONS

The conversion rate of plastic work to heat,  $\beta$ , has been investigated for the alloy Ti-6Al-4V. The MTS model has been shown to predict a variation with plastic strain for  $\beta$  in this alloy. A modification was made to the MTS model to include the effect of initial cold work in the material.

The general form of the MTS model prediction for  $\beta$  compares well with a torsion experimental result. Both the experiment and model show  $\beta$  to increase in value from between 0.3-0.6 at low plastic strains up to around 1.0 at high plastic strains.

An alteration to one of the constants was needed to produce good correlation between model and experimental flow stress. The main cause of this discrepancy was assumed to be differences in interstitial atom concentrations, though other effects such as grain size and texturing could also be responsible.

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