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ANISOTROPY-CORRECTED MTS CONSTITUTIVE STRENGTH MODELING IN HY-100 STEEL

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Introduction

The role of texture and its evolution during deformation is well recognized as affecting macroscopic mechanical response. Recent work has emphasized characterizing and quantifying the effect of texture and its evolution on the yield surface and Taylor factor of deformed polycrystals. Validation of these recent efforts is being conducted through evaluation of the existing constitutive database and attempting to account for apparent disparities between constitutive strength model predictions and experimental data. In particular, the relationship between slip modes and texture evolution on mechanical response in body-centered cubic metals and alloys is being probed to rationalize differences between Mechanical Threshold Strength (MTS) model predictions and experimental mechanical test data.

This study addresses some of these issues by attempting to rationalize the rapid increase in yield strength of a HY-100 steel with decreasing temperature from 298 K to 77 K on the basis of a change in slip behavior from 3-system ({123}<111>, {110}<111> and {112}<111>) or 2-system slip ({110}<111> and {112}<111> systems) to restricted glide ({110}<111>). Although pencil glide slip is traditionally associated with slip at room temperature in many bcc metals and alloys, it will be shown that the essential deformation characteristics of pencil glide can be captured using either 2- or 3-system slip. The results presented illustrate that by compensating for texture and its evolution *via* the Taylor factor for a particular slip mode, very good agreement can be achieved between model prediction and experimental data.

Experimental

The deformation response of a 25 mm-thick plate of quenched-and-tempered HY-100 steel at temperatures of 77 K and 298 K was investigated to quantify the role of slip mode on constitutive response. The HY-100 plate studied has a nominal composition of 0.16C-2.62Ni-1.32Cr-0.25Mo-0.26Mn-0.14Cu-0.22Si-0.008P-0.009S-Bal. Fe, and was received and tested following a quench-and-temper heat treatment. Quasi-static uniaxial compression tests of 6.35 mm (dia.) $\times$ 6.35 mm (length) were performed at a strain-rate of 0.001 s^{-1}.

The quasi-static test data, in conjunction with measured high strain-rate data (reported elsewhere (1) were used to determine material model parameters for the MTS strength model (2). Polycrystalline

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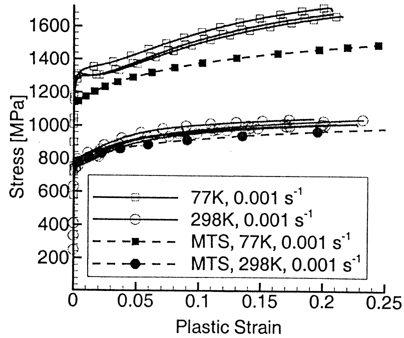

Figure 1. Quasi-static stress-strain response, experimental data and MTS strength model representation, of HY-100 steel at 77 K and 298 K.

plasticity calculations using a modified version of the Los Alamos polycrystal plasticity (LApp) code (3–5) were also performed to calculate slip-mode dependent Taylor factor evolution in order to rationalize differences between the cryogenic and ambient temperature strength data. For more details regarding the experimental and data analysis procedures employed, the interested reader is referred to reference 1.

Results and Discussion

The quasi-static stress-strain responses of HY-100 steel tested at 77 and 298 K are illustrated in Figure 1. Similar to most body-centered cubic (bcc) metals an appreciable increase in the 0.2% offset yield strength (σ_y) is observed with decreasing temperature. Between 298 and 77 K a 500 MPa increase in σ_y is observed, i.e., from ~ 800 MPa at 298 K to ~ 1300 MPa at 77 K. Figure 1 also illustrates that a decrease in test temperature from 298 K to 77 K results in an increase in the hardening rate, ($\theta = d\sigma/d\bar{\epsilon}$), by a factor of three. Specifically, n increases from ~ 600 MPa/strain at 298 K to ~ 2200 MPa/strain at 77 K, at a plastic strain of 0.10.

Also illustrated in Figure 1 are the MTS strength model representations of the quasi-static mechanical responses at 77 and 298K. The MTS strength model equations and parameters for HY-100 steel are discussed in detail in reference 1, but in short are given as:

$$\frac{\sigma}{\mu} = \frac{\sigma_a}{\mu} + \left[1 - \left(\frac{kT}{g_{oi}\mu b^3}\ln\frac{\dot{\epsilon}_{oi}}{\dot{\epsilon}}\right)^{1/qi}\right]^{1/pi} \cdot \frac{\hat{\sigma}_i}{\mu_o} + \left[1 - \left(\frac{kT}{g_{o\epsilon}\mu b^3}\ln\frac{\dot{\epsilon}_{o\epsilon}}{\dot{\epsilon}}\right)^{1/q_\epsilon}\right]^{1/p_\epsilon} \cdot \frac{\hat{\sigma}_\epsilon}{\mu_o}$$

$$\theta = \frac{d\hat{\sigma}_\epsilon}{d\epsilon} = \theta_0\left\{1 - \tanh\left(\alpha\frac{\hat{\sigma}_\epsilon}{\hat{\sigma}_{\epsilon s}}\right)\right\} + \theta_{IV}\tanh\left(\alpha\frac{\hat{\sigma}_\epsilon}{\hat{\sigma}_{\epsilon s}}\right);\ \ln\left(\frac{\dot{\epsilon}_{\epsilon so}}{\dot{\epsilon}}\right) = -\frac{\mu b^3 g_{o\epsilon s}}{kT}\ln\left(\frac{\hat{\sigma}_{\epsilon s}}{\hat{\sigma}_{\epsilon so}}\right);$$

$$\mu = \mu_o - \frac{D}{\exp(T_o/T) - 1} \qquad [1]$$

where σ_a 40 MPa, $\hat{\sigma}_i = 1341$ MPa, $\mu_o = 71460$ MPa, D = 2910 MPa, $T_o = 204$ K, $k = 1.38\times10^{-23}$ J/K, $b = 2.48\times10^{-10}$ m, $\dot{\epsilon}_{oi} = 10^{13}\ s^{-1}$, $g_{oi} = 1.161$, $q_i = 1.5$, $p_i = 0.5$, $\dot{\epsilon}_{o\epsilon} = 1\times10^7\ s^{-1}$, $g_{o\epsilon} = 1.6$, $q_\epsilon = 1$, $p_\epsilon = 2/3$, $\theta_o = 6000–2.0758\times T$ [MPa/strain], $\alpha = 3$, $g_{o\epsilon s} = 0.112$, $\hat{\sigma}_{\epsilon so} = 822$ MPa, $\theta_{IV} = 200$ MPa, and $\dot{\epsilon}_{o\epsilon s} = 1\times10^7\ s^{-1}$. These model parameters were derived from the *as-measured* mechanical (compression) data, and as such do not explicitly account for the role of texture. Thermally activated deformation contributions to yielding are included in the intrinsic (subscript i) term, *viz.*, in the normalized activation energy, g_{oi}. The structure evolution term (subscript ϵ) considers thermally activated strain hardening.

Good agreement between the experimental data and MTS strength model is observed at 298 K. However, a notable difference between model and experiment is observed in the yield strength and strain-hardening response at 77 K. The MTS strength model can be forced to fit the 77 K data, *viz.*, through an appropriate selection of p_i and q_i; however, this procedure would effectively change the generally accepted short-range obstacle description (11) appropriate for most metals and alloys, and as such was not implemented. As will be discussed below, this strength differential and strain-hardening behavior at 77K can be partially rationalized by considering the role of active slip modes (1-system slip versus 2-/3-system slip) and attendant texture evolution on deformation behavior.

The Taylor factor is used to capture the orientation dependence of polycrystal strength from numerous sources of variability. Chief among these are the initial texture, the prescribed deformation path along with its associated texture evolution, and the number and type of operative slip systems available to accommodate that deformation. MTS parameters are typically determined from mechanical tests performed over a range of temperatures and strain rates. The parameters have traditionally been assumed to be independent of the deformation path and material properties, such as texture. In addition, it is also recognized that interpolated or averaged parameters such as g_{oi} may be biased by the majority portion of the temperature-strain rate regime in which the data were collected. Therefore, the MTS model predicted stress-strain response of an otherwise equivalent material may differ from the experimentally determined response if differences exist in initial texture, deformation path (e.g., compression versus torsion), and/or active slip behavior from those encountered during the initial MTS calibration. These differences originate due to the anisotropic mechanical response of the polycrystal and the evolution of this response with plastic strain.

A preliminary method to account for these effects consists of a post-MTS correction factor developed below; an example using HY-100 steel is also given. It is stressed that this approach does not represent a implementation within the MTS framework, but rather an inclusive normalization term incorporating the effects of preferred orientation and anisotropic behavior not currently included in the MTS formulation. However, the methodology does not preclude its implementation within MTS at a future date. In this paper we consider the potential effect of a discrepancy in slip behavior at a temperature of interest that differs from the principal temperature range used to determine the MTS parameters. Although the effect of initial texture and deformation path on MTS predictions may be treated in an equivalent fashion, the current study maintains these conditions constant and focuses solely on the change in slip behavior. As such, identical initial textures and uniaxial compression deformation paths are considered for both the MTS calibration and so-called *current test*. It is essential that the initial texture and deformation path employed during the MTS calibration tests be known, along with an assumed set of slip systems, so that a baseline $M(\epsilon)$ can be computed. The anisotropic behavior associated with the MTS calibration tests, and therefore MTS parameters, is captured in this baseline $M(\epsilon)$.

Polycrystal plasticity calculations suggest the differences in yield strength and strain-hardening rate at 77K between model representation and experiment may be rationalized to a large extent by considering differences in slip mode, e.g., 1-system versus 2-/3-system slip, and changes in material texture with increasing deformation. The Taylor factor and its evolution with plastic strain is used to characterize material texture and slip behavior, and to compensate measured (and calculated) flow stress values for these effects. This procedure was motivated by the work of others (3–6). The approach to data reduction taken herein presumes the effect of specific slip systems on the flow stress be de-coupled from the constitutive response in order to better characterize the role of microstructure on constitutive response. Specifically, the anisotropic nature of slip is compensated for and effectively removed from the flow stress in order to compare apparently disparate deformation behavior at 77 and 298 K. Slip

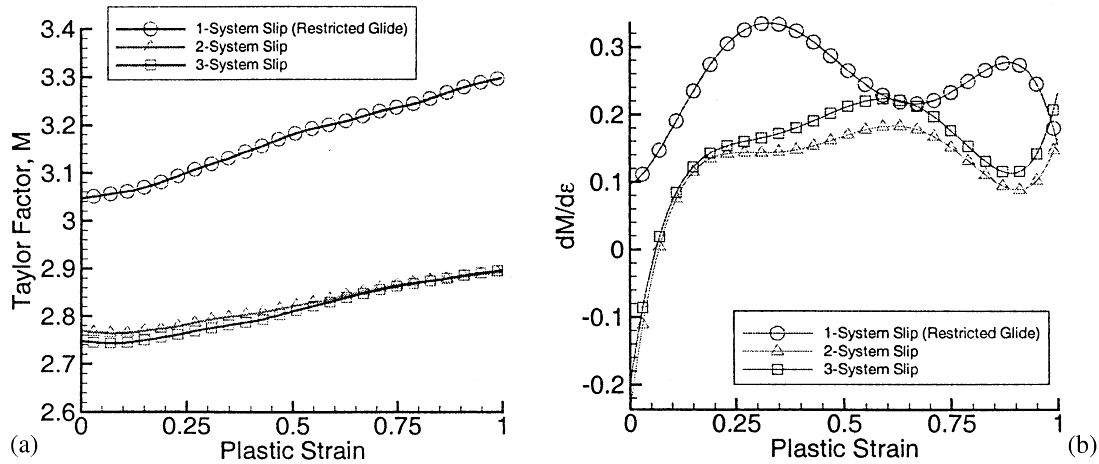

Figure 2. (a) Taylor factor evolutions for 1-system, 2-system, and 3-system slip. (b) Instantaneous derivative of Taylor factors for 1-system, 2-system, and 3-system slip.

mode is de-coupled from the flow stress by normalizing the measured (uniaxial) flow stress at an effective strain by a corresponding normalized Taylor factor associated with that particular strain level, such that:

$$\sigma^*(\epsilon) = \sigma_{MTS}(\epsilon)/\bar{M}(\epsilon) \qquad [2]$$

where σ^* is the anisotropy corrected stress, σ_{MTS} is the MTS-predicted flow stress and $\bar{M}$ is the normalized Taylor factor. The normalized Taylor factor is defined as the ratio of the Taylor factor associated with the prevailing test conditions and the Taylor factor associated with the texture, strain path, and slip behavior encountered during MTS parameter calculations, both as a function of strain:

$$\bar{M}(\epsilon) = M_{Current}(\epsilon)/M_{Baseline}(\epsilon) \qquad [3]$$

where $M_{Current}$ refers to the Taylor factor associated with the current test of interest and $M_{Baseline}$ refers to the Taylor factor associated with the MTS calibration tests. Two- and three-system slip are chosen for the baseline as the constitutive model is calibrated using mechanical data in the temperature range for which these slip systems are assumed to adequately characterize the deformation behavior. As such, in this study Taylor factors for the active slip system are calculated assuming either restricted glide at 77 K or 2-system or 3-system slip at 298 K.

Initial results indicate 2-system and 3-system slip produce essentially identical deformation behavior. Slip mode dependent Taylor factors were calculated with LApp as a function of strain as the initial step to de-couple the effect of the active slip system on deformation; see Figure 2a. For the case of α-iron, as with most bcc metals, low-temperature deformation and alloying promote the restriction of slip to {110}<111> systems (7–9). Therefore, it is presumed that restricted glide characterizes the slip behavior for the HY-100 alloy at cryogenic temperatures, such as 77K. Pencil glide slip is approximated by two-system slip and is assumed to characterize the slip behavior at ambient temperature. Taylor factor evolutions for 1-system, 2-system, and 3-system slip are represented by 6th order polynomials and given as:

$$M(\text{1-system}) = -3.21\epsilon^6 + 8.9446\epsilon^5 - 8.5176\epsilon^4 + 2.7912\epsilon^3 + 0.1467\epsilon^2 + 0.096\epsilon + 3.0466 \qquad [4]$$

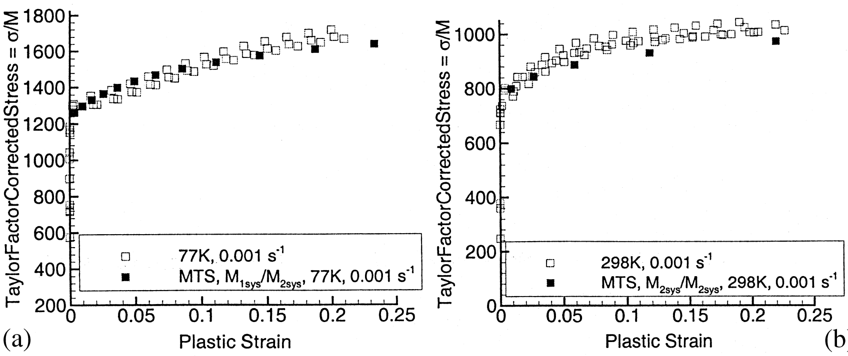

Figure 3. (a) Taylor factor compensated 77 K stress-strain response - comparison between MTS prediction and experimental data (b) Taylor factor compensated 298 K stress-strain response - comparison between MTS prediction and experimental data.

for the case of 1-system slip,

$$M(\text{2-system}) = 3.4437\epsilon^6 - 10.848\epsilon^5 + 13.104\epsilon^4 - 7.7542\epsilon^3 + 2.4125\epsilon^2 - 0.2364\epsilon + 2.7706 \quad [5]$$

for the case of 2-system slip, and

$$M(\text{3-system}) = 3.5961\epsilon^6 - 10.883\epsilon^5 + 12.559\epsilon^4 - 7.1206\epsilon^3 + 2.1975\epsilon^2 - 0.1999\epsilon + 2.7485 \quad [6]$$

for the case of 3-system slip.

Immediately noticeable from Figure 2a is that the Taylor factor is nearly equivalent for 2-system and 3-system slip. Also observed is that the Taylor factor is larger in 1-system slip than in either 2- or 3-system slip. For example, the difference in initial Taylor factors ($M(\epsilon)$ at $\epsilon = 0$) between 1-system and 2-/3-system slip is approximately 13%. A larger value of the Taylor factor results in a higher value of yield strength and flow stress in restricted glide. Secondly, the instantaneous derivative, $dM/d\epsilon$, at comparable strain levels is also larger in 1-system slip than in either 2- or 3-system slip, as illustrated by Figure 2b. This $dM/d\epsilon$ behavior tends to suggest that the "hardening" rate of the Taylor factor, due to different texture evolution, is larger in 1-system slip as compared to 2-/3-system slip. This higher value of Taylor factor hardening is presumed to yield, in part, the higher hardening rate observed at 77 K than at 298 K, assuming similar strain-hardening processes occur at both temperatures. However, the inflection in 1-system slip dM/de response at $\epsilon = 0.35$ is in marked contrast to that illustrated by either 2- or 3-system slip. One-system slip is the analytical solution to the Taylor-Bishop-Hill equation, whereas 2- and 3-system slip are calculated using the LApp code and a newly developed interpolation scheme to determine a so-called *rate-insensitive* Taylor factor (10).

Calculated MTS model flow curves for 77 and 298 K were compensated for slip mode using equation (3). Reiterating, the MTS model predictions incorporating Taylor factor evolutions are normalized by $M_{baseline}$ because the model representation for HY-100 steel is biased toward higher temperatures in which multi-mode slip dominates. Normalized Taylor factors in this case at 77 K are equivalent to $M_{1\text{-}system}(\epsilon)/M_{2\text{-}system}(\epsilon)$, whereas at 298 K they are unity for all values of strain.

Figure 3a illustrates the Taylor factor compensated, MTS predicted stress-strain response of HY-100 steel at 77K and 0.001 s^{-1}. As shown by this figure very good agreement is obtained in the yielding behavior between the 77 K strength model characterization and experimental data, whereas strain-hardening behavior is captured in part. Overall, there is a significant improvement in the compensated MTS prediction as compared to the uncompensated in Figure 1. Figure 3b illustrates the stress-strain curves, experimental and MTS model, for 298 K and 0.001 s^{-1}. As the Taylor factor normalization at 298 K is trivial, the original, uncompensated MTS model characterization is recovered from the normalization procedure, and shows good agreement with experimental results. The effect on Taylor factor from texture evolution for the modest compressive strains imposed for this test is minor compared with the effect from active slip modes.

The implication of the Taylor factor normalization applied to the MTS strength model is that the strength model is biased toward 2-/3-system slip, and that by compensating the strength model by the Taylor factor the predicted and experimental quasi-static mechanical response at 77 K can be brought into agreement. Also, the Taylor factor normalization of the 77 K MTS model prediction tends to indicate that the dominant deformation mechanism at 77 K is characterized within the single "intrinsic" term (subscript i) within the MTS framework. This further suggests that the dominant thermally activated process between 77 and 298 K is related to the original deviation between MTS prediction and experiment attributable to differences in the active slip systems.

Conclusion

A Taylor factor normalization routine was developed for MTS predictions of stress-strain response. This correction accounts for discrepancies between predicted and experimental results arising from anisotropic material response not accounted for within the MTS model, including initial texture, deformation path, and slip behavior. Polycrystal plasticity calculations were used to predict Taylor factor evolution during the deformation event. For the case of a HY-100 steel compression test at 77K, the method resulted in a significant improvement in predicted response.

The active slip systems are found to have a noticeable effect on the predicted flow stress behavior of HY-100 steel and can be compensated through normalization by the Taylor factor. Compensating the 77 K flow stress behavior of HY-100 steel by the Taylor factor evolution characteristic of restricted glide in a bcc material brings into very good agreement the MTS model-predicted and experimental data. Similar agreement is achieved when compensating the 298 K flow stress by the Taylor factor characteristic of 2-/3-system slip (used as an approximation to pencil glide slip). The results of the Taylor factor normalization to the constitutive behavior indicate the dominant thermally activated deformation process can be captured *via* a single Arrhenius-like relationship. In particular, for HY-100 steel thermally activated yielding is captured within a single *intrinsic* (g_{oi}) strengthening term. From a phenomenological standpoint the single "intrinsic" term tends to suggest a common deformation mechanism, possibly the Peierls barrier, dominates at 77 and 298 K.

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