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A constitutive model on flow stress prediction from the contribution of twin and grain refinement, strain and strain rate during surface mechanical attrition treatment of metals

Wing Yan LEUNG, San Qiang SHI, Jian LU, Hai Hui RUAN and Li Min ZHOU
A constitutive model on flow stress prediction from the contribution of twin and grain refinement, strain and strain rate during surface mechanical attrition treatment of metals

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A new constitutive equation is developed to model the flow stress on a metal surface undergone high speed impacts that result in strain hardening. The new equation is based on the Johnson-Cook model and has considered the effects of strain, strain rate, grain refinement, twin formation and twin spacing. Two mechanisms for the strain hardening are proposed: Grain refinement or twin formation, depending on the strain rate. At low strain rate, the Hall-Petch relation is obeyed, while at high strain rate, the flow stress is controlled by the formation of deformation twins. The theoretical estimation of flow stress agrees well with experimental data for stainless steel 304. According to the new model, the flow stress can be as high as 1.46 GPa at a strain rate of 10⁹/s.

Keywords: SMAT, flow stress, grain refinement, twin spacing, metal plasticity.

INTRODUCTION

Researchers have been investigating various manufacture processes to improve mechanical strength of metals (Iwahashi et al., 1996; Kim and Kim, 2010; Ye et al., 2014; Ye et al., 2015). Among these processes, Surface Mechanical Attrition Treatment (SMAT) (Lu and Lu, 1999) has attracted significant interests because this method can create nano-sized grain structures and/or twin structures in metals and alloys such as stainless steels. During SMAT, a surface of a metal is impacted by high-energy rigid balls with random impact directions, which may activate most of dislocation slip systems in crystalline metals. Efforts have been made to develop the relationship between various variables in SMAT process and grain refinement, in order to predict the flow stress in the deformed layer (Zhang et al., 2011). There is clearly a need to be able to predict flow stress when both deformation twin and grain refinement are developed during SMAT.

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Lots of experiments were conducted to investigate the mechanical properties after SMAT (Chen et al., 2007; Li et al., 2009). It was observed that the strain, strain rate, grain size and twin spacing all contribute to the increase of flow stress in the metals through SMAT process. The common constitutive law used in describing metal plasticity was Johnson-Cook Model (JC Model) (Johnson and Cook, 1983, 1985). This model describes the evolution of flow stress as a function of strain, strain rate and temperature during deformation. However, this model does not link the microstructure evolution to the flow stress. Hall-Petch model (Hall, 1951; Petch, 1953) has linked the grain size to yield stress and was used widely.

It was well known that many metal and alloy systems can develop deformation twins during plastic deformation (Chen et al., 2003; Wu et al., 2006; Michiuchi et al., 2006; Kibey et al., 2007; Xiao et al., 2008; Li et al., 2010). For example, Chen et al. (2003) analyzed the critical condition for the formation of deformation twins as compared to nano-crystallization grains in aluminum. Farrokh and Khan (2009) had developed a constitutive model by integrating the Johnson-Cook model with the grain refinement. The objective of this research is to develop a constitutive model that can predict the flow stress with the consideration of the microstructure evolution such as twin spacing and grain size during SMAT.

**DEVELOPMENT OF CONSTITUTIVE EQUATION**

**Assumptions**

The following assumptions are made:

i. The grain size produced in SMAT is greater than the twin spacing.
ii. The deformation twin can only form above a certain strain rate, and twin spacing formed in the hardening process depends only on the equivalent plastic strain.
iii. The minimum grain size is equal to the twin spacing.
iv. The effect of the grain size on flow stress follows the Hall-Petch relationship.

**Elastic-plastic formulation**

Within the model discussed here, J2 plasticity with isotropic hardening is assumed. The elastic and plastic response of the material is defined by (i) yield criterion, (ii) flow rule and (iii) constitutive model (Neto et al., 2008). In the elastic response, the material obeys the Hooke’s law. The trial total strain \( \mathbf{e}^e_{(n+1)} \) and stress \( \mathbf{s}^e_{(n+1)} \) can be updated by:

\[
\mathbf{e}^e_{(n+1)} = \mathbf{e}^e_{n} + \Delta \mathbf{e}
\]

\[
\mathbf{s}^e_{(n+1)} = 2G \mathbf{e}^e_{(n+1)}
\]

\[
(\sigma_m^e)_{(n+1)} = K \mathbf{e}^e_{(n+1)}
\]

Denote

\[
q_l(s) = \sqrt{3}j_2(s)
\]

\[
q^*_{(n+1)} = \frac{3}{2} s^e_{(n+1)} s^e_{(n+1)}
\]

Where the notation with \( (\cdot)^e \) and \( (\cdot)^* \) refer to the elastic system and trial value respectively; \( \mathbf{s} \) refers to the deviator stress; \( \mathbf{e} \) is strain tensor; \( \mathbf{e}^e \) is a sum of \( e_{11}^e, e_{22}^e \) and \( e_{33}^e \); \( G \) and \( K \) are the shear and bulk modulus respectively; \( \sigma_m^e \) is the trial axial stress in one-dimension; and \( (\cdot)_n \) refers to the current time step.

The calculated trial stress \( \sigma^e_{(n)} \), is compared with the yield function, \( \Phi(\mathbf{\sigma},\sigma_f) \), in the following conditions. If it is under elastic deformation, the trial stress is then the updated stress \( \mathbf{s}^e_{(n+1)} \).

\[
\Phi(\mathbf{\sigma},\sigma_f) \begin{cases} < 0 & \text{elastic} \\ \geq 0 & \text{plastic} \end{cases}
\]

Once the material is under the plastic response, the plastic flow rule is applied in form of:

\[
\mathbf{e}^p_{(n+1)} = \mathbf{e}^e_{(n+1)} + \Delta \overline{\mathbf{e}}^p
\]

\[
\sqrt{3} J_2 (s^e_{(n+1)}) - \sigma_f (\overline{\mathbf{e}}^p_{(n+1)}) = 0
\]

Where \( \overline{\mathbf{e}}^p \) is the equivalent plastic strain. The state variables are updated in the following:

\[
\sigma_{m(n+1)} = (\sigma_m^e)_{(n+1)}
\]

\[
\mathbf{s}^e_{n+1} = \left(1 - \frac{3G \Delta \overline{\mathbf{e}}^p}{\overline{\mathbf{e}}^p_{(n+1)}}\right) \mathbf{s}^e_{(n+1)}
\]

\[
\overline{\mathbf{e}}^p_{(n+1)} = e^p_{(n)} + \Delta \overline{\mathbf{e}}^p
\]

**Modification of JC model**

The JC model is the constitutive equation used here for the calculation of flow stress. However, the original model only relates the strain, strain rate and temperature to flow stress of the materials, without considering the effect of microstructure evolution. In this section, the detailed modifications of the original JC model will be presented in relation to the evolution of grain size and twin spacing.
**JC model**

In the JC model, the flow stress is expressed as a function of strain, strain rate $\dot{\varepsilon}$, and homologous temperature $T^{\text{hom}}$, as presented in Equation (11) (Grujicic et al., 2012; He et al., 2013; Wang and Shi, 2013).

$$\sigma_f = (A + B \varepsilon^n)(1 + C \ln \dot{\varepsilon}^s)(1 - T^{\text{hom}})$$  \hspace{1cm} (11)

Where $A$, $B$, $C$, $m$ and $n$ are material constants. The homologous temperature is given by $T^{\text{hom}} = \frac{(T - T_m)}{(T_m - T_c)}$, where $T_c$ is the melting temperature and $T_m$ was the annealing temperature. Since the flow stress is a function of strain, the JC equation represents the plastic deformation induced by strain hardening. If the effect of the material response is mainly determined by the term $(A + B \varepsilon^n)$, the strain rate and homologous temperature may be neglected. The material constant, $A$, could then be determined as static yield stress before strain hardening, that is, $A = \sigma_y$. The parameter A in the JC model represents the static yield stress in elastic response. When the material is under a continuous hardening process, parameter $A$ is no longer a constant. The parameter $A$ is varying with the material response in the development of dislocations. In this condition, the yield stress is dependent on the microstructure evolution and changing with the strain. Thus, the flow stress can then be related to the change of microstructure and macrostructure as well.

**Yield stress**

With strain hardening, the yield stress $\sigma_y$ changes as microstructure changes, such as the increase of dislocation density (Taylor, 1934a, b; Mecking and Kocks, 1981). An effort was made to link microstructure parameters such as dislocation density to the apparent yield stress as:

$$\sigma_y = \alpha G b \rho_G + \rho_{GB} + \rho_{TB}$$  \hspace{1cm} (12)

Where $\rho_G$, $\rho_{GB}$, and $\rho_{TB}$ refer to the dislocation densities inside a grain, at grain boundary, respectively; $G$ is shear modulus; $b$ is the Burger vector; $\alpha$ is a geometric constant. The dislocation density at grain and twin boundaries is much greater than that inside a grain. The total dislocation density may be approximated as:

$$\sigma_y = \alpha G b \rho_G + \rho_{TB}$$  \hspace{1cm} (13)

Dislocation density in twin boundary $\rho_{TB}$: The formation of deformation twins and refinement of grains may happen at the same time for some materials during SMAT. It is assumed that there is a twin boundary dislocation pile-up zone (TBDPZ) at the twin boundary (Zhu et al., 2011). A high density of dislocations is concentrated at this very thin layer. The phenomena are illustrated in Figure 1. The dislocation density at TBDPZ is expressed as Equation 14. The dislocation density is related to twin spacing ($d_{TB}$), which agreed with the observation that the grain size reduction would increase the yield stress.

$$\rho_{TB} = \left(\frac{14}{\pi} \frac{d_{\text{TBDPZ}}}{\rho_{TB}}\right) \left(\frac{1}{\pi} \frac{d_{TB}}{\rho_{TB}}\right) = \left(\frac{1}{\pi} \frac{d_{TB}}{\rho_{TB}}\right) \left(\frac{1}{\pi} \frac{d_{TB}}{\rho_{TB}}\right)$$  \hspace{1cm} (14)

Where $d_{\text{TBDPZ}}$ is the thickness of TBDPZ, $\phi_{TB}$ and $\rho_p$ are geometric factors; $d_{\text{TB}}$ is twin spacing, $\rho_1$ and $\rho_0$ are constant that independent of the twin spacing.

Dislocation density in grain boundary ($\rho_{GB}$): Another region containing high density of dislocations is a grain boundary dislocation pile-up zone (GBDPZ) (Zhu et al., 2011). This region is around the grain boundary as shown in Figure 1 and plays an active role during the plastic deformation in the dislocation development. The dislocation density at the GBDPZ can be calculated by:

$$\rho_{GB} = \frac{n_{\text{GB}} G A}{v_{\text{cell}}} = \frac{6d_{\text{GBDPZ}}}{\phi_b d_G}$$  \hspace{1cm} (15)

Where $n_{\text{GB}}$ is the number of dislocations around the GBs, $\lambda_{\text{GB}}$ is the average length of dislocation loops in GBDPZ ($=\pi d_G$), $d_G$ is the grain size. $v_{\text{cell}}$ is the volume of the unit cell ($=\pi d_G^2$), $d_{GBDPZ}$ is the size of the grain boundary dislocation pile-up zone, $\phi_b$ is the geometry constant in a range of 0.5 to 1.5.

**Modified JC model**

Put Equations 14 and 15 in Equation 13, the yield stress $\sigma_y(d_{TB})$ is:

$$\sigma_y(d_{TB}) = \sigma_y \left(\frac{14}{\pi} \frac{d_{\text{TBDPZ}}}{\rho_{TB}}\right) \left(\frac{1}{\pi} \frac{d_{TB}}{\rho_{TB}}\right) = \sigma_y \left(\frac{14}{\pi} \frac{d_{\text{TBDPZ}}}{\rho_{TB}}\right) \left(\frac{1}{\pi} \frac{d_{TB}}{\rho_{TB}}\right)$$  \hspace{1cm} (16)

From the observations by Chen et al. (2011), a critical strain rate is required for twin formation in stainless steel. When the strain rate is greater than $10^4$ s$^{-1}$, deformation twins will form. While if the strain rate is less than $10^4$ s$^{-1}$, there is no twins formed in stainless steel. At low strain rates, the yield stress is simply determined by the grain size according to the Hall-Petch model. The experimental data were used to determine the material constants in the Hall-Petch relationship for stainless steel 304 (SS304) (Schino and Kenny, 2003a, b; Chen et al., 2011). The yield stress of SS304 $\sigma_y(d_G)$ was determined as:

$$\sigma_y(d_G) = 297 + \frac{57}{\sqrt{d_G}}$$  \hspace{1cm} (17)

The JC equation is finally modified in the consideration of twin spacing and grain refinement

$$\sigma_p = \left[1 + C \ln \dot{\varepsilon}\right] \left[1 - T^{\text{hom}}\right], \dot{\varepsilon} \geq 10^4$$

$$\sigma_p = \left[1 + C \ln \dot{\varepsilon}\right] \left[1 - T^{\text{hom}}\right], \dot{\varepsilon} < 10^4$$  \hspace{1cm} (18)

This new constitutive equation reflects that the flow stress is not only affected by the equivalent plastic strain and strain rate, but also the grain size and twin spacing. The values of those variables in Equations 16 and 18 are given in Table 1.

**Determination of grain size and twin spacing**

The flow stress in the new constitutive equation is now related to
the grain size and/or twin spacing depending on the strain rate. The evolution of grain size and twin spacing are dependent on the equivalent plastic strain during the hardening process.

**Grain size \( (d_G) \) evolution**

In the isotropic hardening process, the grain size is redefined according to the equivalent plastic strain. The refined grain size has been determined by the initial grain size and equivalent plastic strain in Equal Channel Angular Pressing (ECAP) (Kim and Kim, 2010). However, twin formation was not considered.

In the observation by Chen et al. (2011), the increase of equivalent plastic strain \( (\varepsilon^p) \) would lead to the decrease of the grain size when strain rate is low and determined by Equation 19. The grain size \( (d_G) \) can reach the minimum size at 20 nm.

![Figure 1. Illustration of grain and twin boundaries (Zhu et al., 2011).](image)

**Table 1. Parameters used in this work (Chen et al., 2011; Zhu et al., 2011).**

<table>
<thead>
<tr>
<th>( \alpha )</th>
<th>( G )</th>
<th>( b )</th>
<th>( d_{TBDPZ} )</th>
<th>( d_{GRDPZ} )</th>
<th>( n^{\text{GB}} )</th>
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<tr>
<td>0.33</td>
<td>86GPa</td>
<td>0.258nm</td>
<td>3.6nm</td>
<td>3.6nm</td>
<td>( 4 \times 10^6 )</td>
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\[
\eta_1 = 3.5 \times 10^{12} \quad \eta_0 = 2.975 \times 10^6 \quad \eta_p = 0.0367 \quad \phi_{TB} = 0.5 - 1.5 \quad \phi_3 = 0.5 - 1.5 \quad B = 1 \text{GPa} 
\]

<table>
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<tr>
<th>( n )</th>
<th>( C )</th>
<th>( \varepsilon_0^1 )</th>
<th>( m )</th>
<th>( T_0 )</th>
<th>( T_m )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.65</td>
<td>0.07</td>
<td>1.0</td>
<td>1</td>
<td>293K</td>
<td>1500K</td>
</tr>
</tbody>
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When the strain rate is larger than $10^4 \text{s}^{-1}$, the twins formation becomes important in the microstructure evolution. The twins are formed in the grain until the twin spacing is equal to the grain size. At this situation, the grain size is reduced by plastic deformation to be comparable to twin spacing ($d_{TB}$):

$$d_G = d_{TB}$$  \hspace{1cm} (20)

**Twin spacing reduction ($d_{TB}$)**

Once there is twin formation during the hardening process at high strain rate, the evolution of twin spacing is crucial to the flow stress calculation. In this situation, the twin spacing ($d_{TB}$) was affected by the equivalent plastic strain. The experiment conducted by Chen et al. (2011) provided an empirical model to calculate the twin spacing in stainless steel as:

$$d_{TB} = \frac{1}{35e^{0.2P+10}}$$  \hspace{1cm} (21)

Similar to the refinement of grain size, the increase of equivalent plastic strain would lead to the decrease of the twin spacing. The minimum twin spacing was found to be 12.5 nm when the equivalent plastic strain was about 0.088.

**RESULTS AND DISCUSSION**

**Validation of the new constitutive equation**

The new constitutive Equation 18 is now used to predict the flow stress and the results are compared to the experimental results in literature. The twin spacing and grain size measured were approximately 10 and 20 nm, respectively in experiments (Chan et al., 2010). Using the data in Table 1, the yield stress predicted is approximately 1.3 GPa, which compares well to the experimental value 1.2 GPa under the same condition.

**Stress prediction**

The flow stress in SS304 is determined by two mechanisms, grain refinement and twin spacing, depending on the strain rate during the strain hardening. The change of flow stress by these mechanisms are calculated by Equation 18 and compared in Figure 2 with respect to the strain in the impact ($z$-) direction during SMAT. The flow stress by grain refinement is monotonically increasing with the strain. While the flow stress by twin spacing and grain refinement together (blue line) increases to a maximum value and then decreases.

![Figure 2. Comparison of flow stress dominant by grain refinement or twin formation.](image-url)
Further decrease of the twin spacing can no longer increase the flow stress.

Below 0.05 strain, the flow stress due to the grain refinement is greater than that due to twin formation, while at higher strain, the opposite becomes true. The flow stress reaches the maximum value of 1.33 GPa when the twin formation is in effect together with grain refinement.

The variations of flow stress as a function of strain rate are plotted in Figure 3 and 4. The maximum flow stress can be found at 1.46 GPa due to twin formation with a strain rate of $1 \times 10^5$ /s. During SMAT process, the high velocity of ball impact can produce the strain rate as high as $1 \times 10^5$ /s. This prediction is qualitatively consistent to
the experiment observation by Chan et al. (2010).

Conclusion

In this work, both the change of macrostructure and microstructure are considered in the modified Johnson-Cook model. The flow stress is now related to the strain, strain rate, temperature, together with grain size and twin spacing in the presence of deformation twins. The formation of deformation twins is dependent on the strain rate. Thus, the new constitutive equation for the flow stress prediction should be divided into two cases, that is, grain refinement only, or twin formation plus grain refinement. Predictions by this new constitutive model on flow stress compared well to the experimental results for SS304 in which, both microstructure such as grain size and twin spacing, and flow stress were measured. Based on this new constitutive model, the ranges of flow stresses in two cases are predicted. In the presence of deformation twins and grain refinement, the flow stress is 1.33 GPa; while it is 1.13 GPa in the case of grain refinement only at the same strain. Since the incident angle and velocities of the ball affect the energy transmitted to the metal in SMAT, the strain rate of the metal in the impact direction can be as high as $1 \times 10^7$ /s, which results in high flow stress induced by twin formation. It is predicted that the maximum flow stress can reach to 1.46 GPa for SS304.

Conflict of Interests

The authors have not declared any conflict of interests.

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