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COMPUTATIONAL MODELS FOR NUCLEATION, GROWTH, AND COALESCENCE
OF ADIABATIC SHEAR BANDS

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Résumé - On établit des équations pour la vitesse de germination et de croissance des bandes de cisaillement adiabatique. Les fonctions que l'on obtient sont en accord avec les observations expérimentales. Elles dépendent principalement de la diffusivité thermique et de la concentration de la déformation à la pointe d'imperfections s'apparentant à des fissures.

Abstract - Nucleation and growth rate functions for adiabatic shear bands are derived. The derived functions are consistent with experimental observations. They depend primarily on thermal diffusivity and the strain concentration at the tips of crack-like imperfections.

I - INTRODUCTION

A companion paper /1/ reports the development of a subroutine, called SHEAR4, for describing adiabatic shear band kinetics. SHEAR4 requires a nucleation rate function that specifies, on discrete planes in the material, threshold criteria for nucleation and the rate at which the number of bands per unit volume increases after the threshold criteria are met. The nucleation rate function must also specify the band sizes on nucleation.

We must also specify the rate at which the bands grow (extend) after nucleation, and the band "jog," B, the slip accommodated by each band. B is the macroscopic equivalent of the Burger's vector for atomic dislocations.

The nucleation and growth rate functions form the "damage evolution" relations that are required for any internal state variable description of damage. In the following paragraphs we derive the nucleation and growth rate relations that are currently used in SHEAR4.

II - NUCLEATION RATE

The conditions for localization of a planar flow perturbation of infinite extent have been studied, both numerically /2/ and analytically /3/ (also, T. W. Wright and R. C. Batra, personal communication). However, the adiabatic shear bands observed in our experiments are not infinite, but appear to nucleate at points and grow radially outward like macroscopic dislocations with edge and screw components.

To better understand the nucleation process for such bands, we performed the numerical calculation illustrated in Figure 1. SHEAR4 was used in its plasticity mode only (no shear bands were created) to computationally simulate a situation in which a small planar crack-like imperfection was loaded remotely in pure shear across the crack face. Plane strain, zero friction conditions were assumed.

We see from Figure 1 that strain concentrations occur at the crack tips and extend about one crack half-length, R, from the tips. There is a strain-free "dead zone" extending about R/2 from each crack face. For the 4340, RC43 steel properties used in the calculation, when the remotely applied strain in the crack plane was 0.13, the strain magnification at the crack tips was about 2.
Since there is no characteristic size governed by material properties in the calculation, the size of the region of magnified strain at the crack tip, \( r \), is a given fraction of the crack half-length, \( R \), for a given remotely applied strain. This result will hold as long as material rate effects and inertia are negligible.

If the deformation occurs rapidly enough to maintain adiabatic conditions around the crack, the threshold condition for nucleation is that the strain at the crack tips is sufficient to cause the stress to drop. In short, we assume that the nucleation threshold condition for a planar imperfection is identical to the growth (extension) threshold condition.

Figure 2 shows static adiabatic yield curves for three hardnesses of 4340 steel. Under these conditions, most of the material strength has been lost for strains exceeding 1.0 to 1.4, and the stress begins to drop at strains of 0.2 to 0.3. The nucleation threshold condition is thus that the local strain at the crack tip reach 0.2 to 0.3.

Our criterion for adiabaticity is that significant heat cannot flow a distance \( R \) (out of the dead zone) during the loading time of interest. That is, the imperfection must remain thermally autonomous.

To make this requirement precise, refer to Figure 1. The remotely applied strain in the crack plane is approximately given by

\[
\Delta \varepsilon_R \sim \frac{B}{R}
\]  

Furthermore, the remote strain rate is given by

\[
\dot{\varepsilon}_R = \frac{\Delta U}{R}
\]

where \( \Delta U \) is the difference in particle velocity measured from \( R/2 \) above the crack to \( R/2 \) below it.

We now state our criterion for adiabaticity:

\[
\Delta U > v_H
\]

where \( v_H \) is a pseudovelocity of heat flow. That is, if particles on either side of the crack are moving past one another faster than heat can flow between them, adiabaticity will be approximately maintained.

The value of \( v_H \) was derived from analysis of heat flow away from a hot slab, maintained at constant temperature, suddenly placed in contact with a cold material. The well known heat diffusion equation can be examined to determine the pseudovelocity of propagation of a given temperature. If the temperature chosen is one-fourth that of the hot slab temperature, one finds that

\[
v_H \sim \frac{10k}{d}
\]

where \( k \) is the thermal diffusivity and \( d \) is the distance the heat has flowed, i.e., the distance into the originally cold material.

If we now replace \( d \) with \( R \) in Eq. (4), and combine with Eqs. (2) and (3), we obtain for the adiabaticity criterion:

\[
R > \sqrt{\frac{10k}{\dot{\varepsilon}_R}}
\]

Inequality (5) provides information regarding the minimum size of crack-like imperfections that can be nucleated. That is, for the experiments discussed in Ref. 114 the strain rates during nucleation were about \( 10^4 \text{ s}^{-1} \). For steels, \( k \approx 0.1 \text{ cm}^2/\text{s} \), so (5) tells us that cracks smaller than about 0.1 mm will not be nucleated in such experiments. This analysis agrees with observations that the smallest bands seen were about 0.1 mm in extent, and no microscopic nucleation sites were seen.
"Dead Zone" Remote Strain = 0.13

\[
\text{Region of Magnified Strain (Peak Strain } \approx 0.3) 
\]

FIGURE 1 COMPUTATIONAL SIMULATION OF PLANE STRAIN CRACK LOADED IN PURE SHEAR

FIGURE 2 STATIC ADIABATIC YIELD CURVES FOR 4340 STEEL
We next discuss the size distributions of the nucleated imperfections. In our experimental observations of shear band size distributions, we found that they usually approximated the form

\[ N_g = N_0 \exp\left(-\frac{R}{R_1}\right), \]  

(6)

where \( N_g \) is the number of bands per unit volume in a given material plane with sizes greater than \( R \), \( N_0 \) is the total number of bands per unit volume in the plane, and \( R_1 \) is the characteristic size of the distribution.

If a material had an initial distribution of crack-like imperfections given by Eq. (6), Eq. (5) tells us that only those imperfections large enough to satisfy the inequality will be nucleated. However, it is inconvenient to have a lower size cutoff during nucleation in SHEAR4, and as we shall see later, the smallest bands will grow very slowly. Therefore, we simply let \( R_1 \) be the "adiabatic limit size" from (5):

\[ R_1 = \sqrt{\frac{10k}{\varepsilon_R}}, \]  

(7)

and we nucleate the bands with the distribution given by Eq. (6).

Another problem with Eq. (6) is that it produces a few very large bands upon nucleation. Such large bands are not observed experimentally unless correspondingly large imperfections are initially present. Therefore, SHEAR4 contains an upper cutoff for the imperfection size, \( R_{\text{max}} \). For values of \( R > R_{\text{max}} \), \( N_g \) is set to zero. \( R_{\text{max}} \) must be determined experimentally.

We now are in a position to derive the nucleation rate function. We begin by writing

\[ \dot{N} = \frac{\text{Number of available nucleation sites}}{\text{Incubation time}}, \]

\[ \frac{N_0 f - N}{\tau}, \]  

(8)

where

\[ \dot{N} = \text{number of bands nucleated per unit volume per unit time} \]

\[ N_0 = \text{density of nucleating imperfections} \]

\[ f = \text{fraction of } N_0 \text{ that can become nucleation sites} \]

\[ \tau = \text{incubation time}. \]

Thus,

\[ N_0 f - N = \text{current density of nucleation sites}. \]

If the nucleating imperfections are widely spaced so no interaction between them is possible, then \( f = 1 \). However, if there is a high density of nucleating imperfections, band autonomy requires that the bands be spaced at least one heat flow spacing apart; i.e., the closest possible band spacing is given by the minimum from inequality (5):

\[ \text{Minimum spacing} = \sqrt{\frac{10k}{\varepsilon_R}}. \]

If the bands are spaced with the above minimum spacing, the volume per band is on the order of \((10k/\varepsilon_R)^{3/2}\). Thus, the density of bands with minimum spacing is on the order of \((\varepsilon_R/10k)^{3/2}\).
To cover both widely spaced and closely spaced nucleating imperfections, we take
\[ f = \text{Min} \left[ \left( \frac{\xi_R}{10k} \right)^{3/2} / N_o, \ 1 \right] \]  
(9)

We next estimate the incubation time, \( \tau \). Referring again to Figure 1, we see that
the local strain rate at the crack tip can be written
\[ \dot{\varepsilon}_L = M \dot{\varepsilon}_R \]  
(10)

where \( M \) was about equal to 2 in the example calculation. We estimate the incubation
time to be the time required to bring the crack tip strain to the completely
softened value, \( \varepsilon_m \) (1-1.4 for 4340 steel), from the nucleation value, \( \varepsilon_{cr} \). Thus
\[ \tau \approx \frac{(\varepsilon_m - \varepsilon_{cr})}{M \dot{\varepsilon}_R} \]  
(11)

where \( \varepsilon_{cr} \) is the adiabatic strain at which the stress begins to drop.

Values of \( \varepsilon_m - \varepsilon_{cr} \) can often be obtained from thermal softening data in handbooks.
However, a rough estimate can be obtained from the formula
\[ \sigma_y (\varepsilon_m - \varepsilon_{cr}) \approx \rho E_m \]  
(12)

where \( \sigma_y \) is the yield strength at the onset of nucleation, \( \rho \) is the density, and \( E_m \) isthe specific melt energy. Since \( \rho \) and \( E_m \) are easily available material proper-
ties and since Eq. (11) is only approximate in any case, we replace (11) with
\[ \tau = \frac{\rho E_m}{\sigma_y M \dot{\varepsilon}_R} \]  
(13)

We now combine Eqs. (8), (9), and (13) to obtain the nucleation rate function:
\[ \dot{N} = \frac{\sigma_y}{\rho E_m} M \dot{\varepsilon}_R \left[ \left( \frac{\xi_R}{10k} \right)^{3/2} - N \right] H \left( \varepsilon_R - \frac{\xi_{cr}}{M} \right) \]  
(14)

for closely spaced nucleation sites, i.e., \( \left( \frac{\xi_R}{10k} \right)^{3/2} / N_o < 1 \), and

\[ \dot{N} = \frac{\sigma_y}{\rho E_m} M \dot{\varepsilon}_R \left[ N_o - N \right] H \left( \varepsilon_R - \frac{\xi_{cr}}{M} \right) \]  
(15)

for widely spaced nucleation sites, i.e., \( \left( \frac{\xi_R}{10k} \right)^{3/2} / N_o > 1 \), where
\( H \left( \varepsilon_R - \frac{\xi_{cr}}{M} \right) \) is a Heaviside function.

III - GROWTH RATE

To derive the adiabatic shear band growth rate used in SHEAR4, we refer again to
Figure 1. We now interpret the crack-like imperfection in the figure as a nucleated
shear band. The criteria for band growth (extension) are that adiabaticity be
maintained and that the strain at the band tip attains \( \varepsilon_m \). The time to reach \( \varepsilon_m \) is
the incubation time from Eq. (11). The growth rate is thus
\[ \dot{R} = \frac{r M}{(\varepsilon_m - \varepsilon_{cr})} \dot{\varepsilon}_R \]  
(16)

where \( r \) is the size of the magnified strain region at the band tip. As discussed
earlier, in the absence of material rate effects or inertial effects, \( r \) is
proportional to \( R \):
\[ r = B R \]  
(17)
Thus, (16) becomes
\[
\frac{\dot{R}}{R} = \frac{B\dot{M}}{\left(\varepsilon_m - \varepsilon_{cr}\right)} \varepsilon_R
\]  
(18)

The values of \(\beta\), \(M\), \(\varepsilon_m\), and \(\varepsilon_{cr}\) are material properties and must come from analyses or numerical simulations like that of Figure 1. From that calculation, we estimate
\(\beta \approx 1\)
\(M \approx 2\).

As discussed earlier, \(\varepsilon_{cr} \approx 0.2\), \(\varepsilon_m \approx 1\).

Thus, for 4340 steel, Eq. (18) becomes
\(\frac{\dot{R}}{R} \approx 2.5 \varepsilon_R\)  
(19)

This expression is expected to hold until inertial effects become important. At that point, SHEAR4 limits the band velocity to the Rayleigh wave velocity. Recent work by Wu, Toulios, and Freund /4/ also suggests a wave velocity limit.

IV - SIZE OF JOG, B

From Figure 1 we obtained Eq. (1):
\(\Delta \varepsilon_R \approx B/R\)

We can also rewrite Eq (10) as
\(\Delta \varepsilon_L = M \Delta \varepsilon_R\),
where \(\Delta \varepsilon_L\) is the local strain at the band tip. The threshold condition for band nucleation and growth is
\(\Delta \varepsilon_L = \varepsilon_{cr}\).  
(20)

Thus,
\(\Delta \varepsilon_R = \frac{B}{R} = \frac{\varepsilon_{cr}}{M}\),
or \(B \approx (\varepsilon_{cr}/M)R\)  
(21)

This linear dependence of the jog, \(B\), on band length, \(R\), was observed in the experiments discussed in Ref. /1/.

V - DISCUSSION

The derived nucleation and growth relations are approximate and can only serve as starting points for iterative computations with SHEAR4 to simulate experimental results. Nevertheless, comparisons with experimental data show reasonable agreement not only for the form of the equations, but for the numerical values as well. Table 1 shows compares the derived and experimentally determined SHEAR4 parameters from controlled fragmenting cylinder experiments described in Ref. /1/.
### Table 1

**COMPARISON OF DERIVED AND EXPERIMENTALLY DETERMINED SHEAR4 NUCLEATION AND GROWTH PARAMETERS FOR 4340 STEEL EXPANDING CYLINDER EXPERIMENTS**

<table>
<thead>
<tr>
<th>Variable</th>
<th>Value Experimentally</th>
<th>Value Derived</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Determined with Interactive SHEAR4 Simulations [Ref. /1/]</td>
</tr>
<tr>
<td>$R_1$ (nucleation size parameter)</td>
<td>0.01 cm</td>
<td>0.01 cm ($\dot{\varepsilon} = 10^4$ s$^{-1}$)</td>
</tr>
<tr>
<td>$\varepsilon_R$ (nucleation threshold)</td>
<td>0.24</td>
<td>$\varepsilon_{cr}$ $\sim \frac{0.2}{2} = 0.1$</td>
</tr>
<tr>
<td>$B/R$ (ratio of jog to band length)</td>
<td>0.07</td>
<td>0.1</td>
</tr>
<tr>
<td>$\frac{\beta M}{\varepsilon - \varepsilon_{cr}}$ (growth coefficient)</td>
<td>60</td>
<td>2.5</td>
</tr>
</tbody>
</table>

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**REFERENCES**


