Three dimensional structure model of damage in brittle polycrystalline materials
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Abstract

An elementary discussion is presented about the development of microcracks and resulting macroscopic crack extension behavior in brittle polycrystalline materials in connection with three dimensional distribution of intrinsic thermal stress. A simple model was prepared on the basis of finite element method for the evaluation of grain by grain stress distribution. It was revealed that polycrystalline materials have characteristic three dimensional distribution of intrinsic stress, and the macroscopic crack extension resistance would be controlled by resulting three dimensional structures of damage which might be missed by two dimensional analysis. As an example, numerical simulations of macroscopic crack extension were carried out, and the three dimensional result was different from the two dimensional case. It was concluded that three dimensional interpretation is necessary to understand correctly the macroscopic crack extension behavior of brittle polycrystalline materials.

1 Introduction

The toughness of polycrystals, even in the case of single phase ceramics such as alumina, is usually much tougher than that of the constituent single crystals. This effect may be one of the most basic characteristics
of brittle polycrystalline materials, but its mechanism has not yet been fully quantitatively recognized.

Until now, discussion has been mainly focused on two dimensional explanation of the toughness manifestation mechanism in polycrystalline brittle materials. Kim et al.\textsuperscript{2,3} recently pointed out that three dimensional analysis would be necessary for the comprehension of macroscopic toughness of polycrystalline materials. In spite of highly three dimensional grain structure of polycrystalline materials, few reports are found in which the macroscopic crack extension resistance is simulated in connection with three dimensional development of microscopic cracks.

On the other hand, Fu and Evans\textsuperscript{4} analyzed two dimensional thermal stress distribution in polycrystalline ceramic materials of crystal grains with thermal expansion anisotropy and discussed its effect on the development of microcracks on grain boundaries. Due to the high sintering temperature and subsequent cooling, most of ceramics suffer self-equilibrium intrinsic stress inside. Three dimensional intrinsic stress distribution makes non uniform stress distribution along the macroscopically two dimensional through-the-thickness crack front. This variation of stress in the thickness direction will result in a three dimensional structure of microcrack distribution even if all grain boundaries have an identical strength, and might lead to control the macroscopic crack extension resistance. Two dimensional approximation with the stress averaged in the thickness direction would miss this kind of mechanism in the interpretation of macroscopic fracture toughness.

In these circumstances, we here try to present a brief discussion about the development of microcracks and macroscopic crack extension behavior in brittle polycrystalline materials in connection with three dimensional distribution of thermal stress. A simple model is prepared in connection with finite element method for the evaluation of grain by grain thermal stress distribution. Numerical simulation of the initial stage of macrocrack extension is carried out as a first trial, aiming at quantitative estimation of crack extension behavior.

## 2 Stress Distribution and Development of Microcracks along the Macroscopic Crack Front

Let us first simply examine the effect of three dimensional thermal stress distribution on the macroscopic crack extension behavior. Schematic illustration of a brittle polycrystalline material with a through-the-
thickness crack is presented in Figure 1. The lower left side of Figure 1 is the magnified view of the macroscopic crack front, where each crystal grain just ahead of the front is represented by an identical cube. Attention is now focused on an arbitrary grain boundary facet along the front indicated as A, which is coplanar with the crack.

When a microcrack appears on the facet, a part of energy will be released. The amount of released energy could be roughly estimated as equal to the energy released when a penny shaped crack with the same area appears in an infinite elastic body loaded by the stress on the facet, $\sigma$. For simplicity, $\sigma$ is supposed to be applied only in the direction perpendicular to the crack. Then, the average energy release rate $G_1$ with respect to the development of this facet crack would be expressed in the following equation.

$$G_1 = \frac{4d}{3\pi E'} \sigma^2$$  \hspace{1cm} (1)

where $d$ means the equivalent diameter of a penny shape crack and $E'$ is Young's modulus of plain strain. Taking account of the thermal stress, $\sigma$ should be considered to consist of mechanical stress, $\sigma_m$, and thermal stress averaged over the facet, $\sigma_t$. In the absence of thermal stress, $\sigma_m$ may be represented by the stress in the vicinity of a two dimensional crack tip averaged over the length $d$ as

![Figure 1: Schematic model of a macroscopic crack in a polycrystalline material](image-url)
In the above equation, $K_{lm}$ is the macroscopic stress intensity factor; suppose that the crack is loaded in mode I. In the case that the thermal stress $\sigma_t$ is superimposed, $\sigma$ in eqn(1) is replaced with $\sigma_m + \sigma_t$, for the estimation of energy release rate. On the basis of fracture mechanics, the facet crack appears when $G^*$ in eqn(1) reaches to a critical value $G_C$, which is written as in the following equation:

$$G_C = \frac{4d}{3\pi E'} \left( K_{1m} \sqrt{\frac{2}{\pi d}} + \sigma_t \right)^2$$  

By solving eqn(3) with respect to the stress intensity factor $K_{1m}$, we obtain the apparent fracture resistance for a facet to break as

$$K_{1m} = \frac{\pi}{2} \sqrt{\frac{3E'G_C}{2} - \frac{\pi d}{2}}$$

Note that the average thermal stress on the grain boundary facet should be different from one facet to another, because, e.g., the axes of crystal grains with thermal expansion anisotropy may be oriented in a random way. Equation (4) suggests that the external mechanical load required to make a facet crack will vary along the macroscopic crack front even if the strength of each facet is identical, which will lead to the development of a three dimensional structure of microcrack distribution and might control the macroscopic crack extension behavior. In addition, the second term in eqn(4) depends on the equivalent size of penny shaped crack, i.e., the grain size. Vekinis et al.\textsuperscript{5} made a detailed research about the crack extension behavior of alumina ceramics with different grain sizes. They reported that the R-curve behavior (the increase in apparent toughness as the crack grows) showed significant dependence on the grain size, where larger grain size resulted in higher steady state apparent fracture toughness. This fact is in agreement with what eqn(4) means, where larger grains would cause larger variation in $K_{1m}$ and might result in a more complex structure of damage in the process zone ahead of a macroscopic crack.

The mechanism mentioned above might be one of the important factor to comprehend the crack extension behavior of monolithic polycrystalline ceramics, which two dimensional approximation with the stress averaged in the thickness direction would miss. In the following
sections of this paper, as the first trial, we examine the three dimensional character of intrinsic thermal stress based on an elementary model of numerical calculation, setting our sight on a large scale quantitative simulation of crack extension behavior in the future.

3 Evaluation of Three Dimensional Stress

3.1 Numerical modeling of polycrystalline material

In this study, polycrystalline material is numerically modeled as a group of Voronoi polyhedra which represent the constituent crystal grains. Each polyhedron is then divided into tetrahedra by setting their vertices at the center of the polyhedron itself and at the center of every facet, in addition to the original vertices of the polyhedra. In this way, an arbitrary

![Finite element model of crystal grains](image)

Figure 2: Finite element model of crystal grains

<table>
<thead>
<tr>
<th>Material constant</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Young’s modulus</td>
<td>400 (GPa)</td>
</tr>
<tr>
<td>Poisson’s ratio</td>
<td>0.23</td>
</tr>
<tr>
<td>Cooling range</td>
<td>-1130 (K)</td>
</tr>
</tbody>
</table>

Thermal expansion coefficients

\[
\begin{align*}
\alpha_a &= 8.3 \times 10^{-6} \text{ (K}^{-1}) \\
\alpha_b &= 8.3 \times 10^{-6} \text{ (K}^{-1}) \\
\alpha_c &= 9.0 \times 10^{-6} \text{ (K}^{-1})
\end{align*}
\]
Voronoi polyhedron can be automatically divided into tetrahedra. Then, by using these tetrahedra as constant strain elements, a finite element model of polycrystals is developed for the calculation of stress and strain as shown in Figure 2, where adjacent two tetrakaidecahedron shaped crystal grains are representatively presented.

As an example, we consider the intrinsic thermal stress in alumina ceramics. Material constants used for the calculation are presented in Table 1. Note that the thermal expansion coefficient has a different value in one direction of crystal axes, $\alpha_c$, along the c-axis, while the anisotropy of elastic constants is weak and here regarded as an isotropic material.

3.2 Grain boundary stress

We demonstrate in this section some nature of three dimensional thermal stress in comparison to the two dimensional case. Now attention is focused on a grain boundary facet of two adjacent grains as indicated by A in Figure 2. Suppose that these two crystals are inside an infinite body of a polycrystalline material. For the calculation of three dimensional stress, the two grains of interest are set at the center of a cubic domain made up of a sufficient number of the same tetrakaidecahedron shaped grains which are prepared in the way as described above. For a comparison with the two dimensional case, a thin plate model filled with a sufficient number of regular hexagonal grains is used. Thermal expansion coefficients of grains surrounding the two grains under consideration are simply set to be the average of randomly oriented grains, which is equal to $\alpha = (\alpha_a + \alpha_c)/2$ in two dimensional consideration as used in the literature mentioned above. In the case of the three dimensional space, the average coefficient should be $\alpha = (\alpha_a + \alpha_b + \alpha_c)/3$. While the orientations of c-axes in the two grains are set in every direction, stress on the facet is evaluated as the average stress in the elements in touch with the facet. The maximum and minimum values of stress normal to the crack are presented in Table 2.

<table>
<thead>
<tr>
<th>Table 2: Maximum and minimum grain boundary stresses</th>
</tr>
</thead>
<tbody>
<tr>
<td>Max (MPa)</td>
</tr>
<tr>
<td>2 dim</td>
</tr>
<tr>
<td>3 dim</td>
</tr>
</tbody>
</table>
The maximum tensile stress is obviously larger for the case of three dimensional calculation.

With a certain combination of c-axis orientations in the neighboring grains, an interesting distribution of grain boundary stress can also be found as shown in Figure 3. In Figure 3, adjacent grain boundaries perpendicular to each other suffer tensile and compression stresses. Such microscopic stress distribution will lead to a highly three dimensional structure which may be expected to control the macroscopic crack extension behavior.

4 Simulation of crack extension behavior

With the discussion in the previous sections in mind, we tried to carry out an elementary simulation of macroscopic crack extension behavior in a three dimensional polycrystalline brittle material. As an example, transgranular macroscopic crack extension due to the accumulation of grain boundary facet cracks ahead of a through-the-thickness crack is here considered on the basis of the numerical model presented above.

A small region in the neighborhood of a macroscopic crack tip is modeled as shown in Figure 4. In the lower left side of Figure 4, a part of the three dimensional model is teared off so as to show the inner grain structure. For comparison, a two dimensional model made up of hexagonal prisms is also prepared as shown in the lower right side of

![Figure 3: Three dimensional distribution of grain boundary stress](image)

Figure 3: Three dimensional distribution of grain boundary stress
Figure 4. The axis of thermal expansion anisotropy is randomly set in each constituent crystal grain. This region is now supposed to be loaded in mode-I by the macroscopic stress intensity factor $K_{1m}$. Two dimensional elastic displacement field corresponding to $K_{1m}$ is applied to the boundaries of these models.

The energy release rate with respect to the facet cracking is estimated based on eqn(1) where $\sigma$ is evaluated as the average stress in the finite elements in touch with the facet as discussed in the previous section. Taking account of the general state of stress, mode-II and mode-III components of energy release rate, $G_{II}$ and $G_{III}$, corresponding to the shear stress are also considered here. Grain boundary facet cracking is supposed to take place when the total of these three components reaches to a critical value which may be twice the surface energy of grain boundary, $2\gamma_s$.

Then, a facet which satisfies this cracking condition with the minimum value of $K_{1m}$ should be found among all the grain boundaries, and the node at the center of that facet is doubled to introduce a
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microcrack surface into the model. By repeating this procedure, the development process of facet cracks is simulated. When facet cracks accumulate, the node surrounded by facet cracks is also separated to simulate the macroscopic crack extension. The applied boundary displacement field is also moved along with the position of the extended crack tip, which is determined for the three dimensional case as the average position of microscopic zigzag crack front made up of facet cracks being connected to the original through-the-thickness crack. For the simulation, the same constants are used as presented in Table 1, and the surface energy $\gamma_s$ is set to be 1 J/m$^2$.

![Figure 5: Simulated fracture resistance curve](image)

(a) At $a$ in Figure 5 (b) At $b$ in Figure 5

![Figure 6: Simulated appearance of grain boundary facet cracks](image)
Figure 5 shows the simulated curve of crack extension resistance. Macroscopic stress intensity factor $K_{1,m}$ is plotted against the macroscopic crack extension, i.e., the distance, measured in the direction parallel to the original crack, between the original crack tip and the tip of extended crack as determined above. As seen in the figure, the three dimensional result has a trend to increase with respect to the crack extension, while the two dimensional result shows a mere oscillating behavior. The simulated appearance of facet cracks at the positions indicated as a and b in Figure 5 are also presented in Figure 6.

The total crack extension length simulated by three dimensional model might be small, which is due to the restrictions imposed by the computer, and may not be enough to make further discussion at present. However, it is expected that the three dimensional interpretation has essential difference from the two dimensional one. Three dimensional approach will be necessary to understand correctly the crack extension behavior of brittle polycrystalline materials, which will lead to the possibility in the future to control the toughness of monolithic ceramics.

References


