Cohesive Zone Modeling of Grain Boundary Micro-cracking in Ceramics

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Abstract: Finite element methods are used to analyze the micro-structural level thermal anisotropy induced residual stresses of ceramics. The 2D-four-grain model originally proposed by Clarke combined with a damage mechanics based cohesive zone model approach, has been utilized to simulate the grain boundary micro-cracking initiation and arrest due to residual stresses in titanium diboride (TiB\textsubscript{2}). A quantitative relation between the microcracking and grain boundary parameters has been established.

Keywords: Cohesive zone model, residual stresses, titanium diboride

Mathematics Subject Classification: 74R05, 74S05, 74E10, 74F05

1. Introduction

Micro-cracking in ceramics strongly influences their mechanical properties. Micro-cracking arises in ceramics especially along grain boundaries due to the thermal anisotropy of the grains. Thermal expansion anisotropy manifests when the material is subjected to cooling from the fabrication temperature to the room temperature by building up residual stresses. Grain boundaries become available sites for cracking. The existing model by Clarke \cite{1} combined with the use of damage mechanics based cohesive zone model have been utilized to analyze the problem. Critical relations among the involved micro-crack’s parameters are investigated and established.

2. Modeling and material parameters

Material parameters relevant to this study, referred to titanium diboride (TiB\textsubscript{2}), have been taken from Munro \cite{2}. The Young’s modulus $E$ is a decreasing function of temperature. The Poisson’s ratio $\nu$ is kept constant to 0.108. The thermal expansion coefficients $\alpha$ in the crystal directions are increasing functions of temperature, $T$. Dependences on other parameters, if there are any, have been neglected. A single phase, non-textured and defect-free material is considered. A starting temperature of 1500°C is assumed and the cooling is stopped at a temperature of 20°C. The difference of temperature is taken as the load parameter in this analysis. Clarke’s 2D four-grain model simplifies the shape of grains to squares: four grains are surrounded by the rest of the material. The latter will be from now on referred to as the matrix material, which is considered to be elastically and thermally isotropic. The matrix will be assumed to have the average properties of TiB\textsubscript{2}. Each grain is elastically isotropic, with the same $E$ and $\nu$ of the matrix material characterizing the elastic behavior, and thermally anisotropic, with different thermal expansion coefficient in different directions. The directions $\pm 45^\circ$, with respect to the x-axis, are chosen as the ones of maximum/minimum expansion for the upper right grain of the ensemble. The other grains have the same directions of expansion, symmetrically with respect to the axes and the origin. Plane stress

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conditions are assumed. The reference system is taken with the origin in the center of the 4 grains ensemble.

![Diagram](image)

Figure 1 The four grains ensemble surrounded by the matrix, and the FEM model consisting of one quarter of Clarke’s model and surrounding matrix material

ABAQUS has been used to analyze the problem. The finite element model takes advantage of the geometry and material symmetries and considers only one grain, surrounded by matrix material. The finite element model consists of about 18000 elements. The cohesive elements are located along the x-axis and they have a special behavior, described by a traction-separation law [3]. The most relevant parameters identifying the damage and fracture process are: a critical traction value, $\sigma_0$, corresponding to the condition at which the material begins to deform permanently; and the grain boundary energy density, $G_c$, i.e. the energy required for the separation of the material and the creation of the two crack surfaces. A simplified cohesive law has been chosen according to the discussion in [4] for brittle materials. The traction-separation law’s shape is believed to be of less influence on the results [3]. The stress component of interest is the one acting as an “opening” stress along the grain boundary, which is the location for possible cracking [5]. The term ‘opening stress’ means the stress acting to separate two neighboring grains.

3. Results

The first relevant result concerns the thermal anisotropy induced residual stress field in the y direction, $\sigma_{22}$, along the x-axis. Results in Fig.2a show that $\sigma_{22}$ increases with the decrease of temperature. A tensile part and a compressive one are present. At different temperatures the stress re-distributes but maintains the two distinct regions. The position where stress shifts sign is constant for all the temperatures. Fig. 2b plots the opening stress distribution at room temperature.

![Graph](image)
Figure 2: a) Opening stress $\sigma_{22}$ distribution along the x-axis in the grain for different temperatures, grain size $l=50\mu m$, $G_c=0.03N/mm$; b) Stress distribution at $T=20^\circ C$, $l=50\mu m$, $G_c=0.03N/mm$: zoom near the model origin.

Figure 3: Opening stress $\sigma_{22}$ in $x=0$ during the cooling process, grain size $l=50\mu m$, $G_c=0.025N/mm$.

The stress evolution during the cooling process at the origin of the model is plotted in figure 3. It is normalized by the critical stress defined in the cohesive model. After a linear increase with decreasing temperature, the critical stress is reached and the damage starts: the stress decreases slowly to zero, value at which material separation occurs.

Figure 4: Crack size versus grain boundary energy density, grain size $l=50\mu m$.

For a given cooling temperature range, micro-crack initiation and length depend on grain size and grain boundary energy. Figure 4 shows the predicted micro-crack size as a function of grain boundary energy density for a grain size of 50$\mu m$ with a temperature range of $\Delta T=-1480^\circ C$. Fig. 4 shows that the crack size increases for a decreasing value of grain boundary energy density. It is interesting to note that the relation between crack size and grain boundary energy density appears to be almost linear. The most interesting value of grain boundary energy density is the one corresponding to zero crack length. This is a value of great importance to designing micro-crack free materials. The present results have been found to agree well with the experimental [2] and theoretical observations [5].
4. Discussion and Conclusions

A damage-mechanics based cohesive-zone model approach has been developed to analyze the thermal anisotropy induced micro-cracking. The predicted critical grain size for TiB$_2$ seems to well agree with the experimental results in [2].

A quantitative relation between crack size and grain boundary energy density has been established for a given grain size. It has been found that the micro-crack length is linearly related to the boundary energy density. It should be noted that the predicted micro-crack length is slightly influenced by the critical traction value of the cohesive law. Decreasing the value of the critical stress will decrease the final micro-crack length at room temperature.

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References


