Effect of pore morphology on elastic, heat conduction and thermal shock fracture behaviors of porous ceramics

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Abstract

In this study, four different porous microstructures were modelled and simulated using a random algorithm and a three-dimensional finite element method. The effect of pore morphology on the elastic modulus and thermal conductivity of the porous ceramic was investigated, and their possible roles in determination of thermal shock induced stress were studied using the results of finite element simulations. Finally, the relationships between the porous microstructure and their thermal shock cracking resistance were discussed, in terms of pore shape and pore morphology.

Keywords: Porous materials; thermal shock fracture; finite element method;

1. Introduction

Porous ceramics have been widely used in a variety of industrial fields such as heat insulators, catalyst supports, radiant burners and filters for hot gases and molten metals [1-3]. In these applications, the thermal shock cracking and thermal shock induced fracture have constitute a fashionable area of research, because theses properties are closely related to the reliability of such materials in high-temperature engineering applications [4,5].

A common measure of thermal shock resistance of brittle materials (e.g. glass and ceramics) is the maximum thermal gradient which a material can sustain without thermal cracking and/or degradation of stiffness [4,5]. Previous studies have shown that the thermal shock resistance of a material depends on a number of material properties including the fracture strength, elastic modulus, Poisson’s ratio, thermal expansion coefficient, thermal conductivity, and upon the additional parameters such as specimen size and test conditions [6-8]. According to the critical thermal stress criteria proposed by Kingery [6], the high fracture strength, thermal conductivity and the low elastic modulus will bring a good thermal shock resistance. Unfortunately, it is yet unclear whether a porous ceramic has superior or inferior thermal shock resistance to that of a fully dense ceramic, since the elastic modulus and thermal conductivity of these materials are generally both reduced by presence of porosity [9].

On the other hand, thermal shock induced stress in porous ceramics may be influenced significantly by their pore morphologies, because the elastic and thermal properties of this kind of materials depend on the geometrical nature of their microstructure. Additionally, different pore morphologies may lead to different stress states at micro scale due to the difference in local stress concentration near pores. A detailed understanding of the relationships between pore morphology and their thermal shock resistance is therefore required to design and development of the porous
ceramic materials. To the best knowledge of the authors, modelling study of this issue is still not available in the literature.

With this background in mind, this study aims to investigate the effect of pore shape on thermal shock fracture behaviors of porous ceramic materials. A micromechanical modelling of ceramic microstructures under a thermal loading is presented to assess microscopic thermal stress responses of these materials. Representative volume elements (RVEs) of four types of idealized porous microstructures were generated using a random sequential adsorption (RSA) algorithm and their macroscopic elastic modulus, Poisson’s ratio and thermal conductivity were examined using finite element method (FEM). The microscopic and microscopic thermal stresses under a thermal loading were then evaluated using FEM, in terms of pore morphology and their macroscopic elastic and thermal properties.

2. Modelling Porous Microstructures

As inputs for the FEM simulations, four different microstructural models were used which should broadly cover the types of morphologies observed in real porous ceramics. The geometries of the models were generated based on randomly placed spherical pores, solid spheres and ellipsoidal pores. The pore morphologies used for the three-dimensional FEM simulations for elastic, thermal and thermal shock induced stress analyses are shown in Fig.1. They can be characterized as follows:

(1) Isolated spherical pores-Model A (Fig.1a),
(2) Overlapped spherical pores-Model B (Fig.1b),
(3) Overlapped spherical solids-Model C (Fig.1c) and
(4) Overlapped ellipsoidal pores-Model D (Fig.1d).

For the models, a Cartesian coordinate system, \(x, y, z\) was used, and the pores were assumed to be uniformly and randomly distributed in the microstructure. The RVE approaches [10] were used to model the microstructures of porous microstructures with different pore morphologies. The RSA algorithm for creating RVEs of the microstructures consisted of adding pores or solids sequentially into the periodic cubic space by randomly generating the center point \(C(x,y,z)\) of each pores or solids. In the case of Model D, isotropically oriented overlapping oblate ellipsoidal pores, which were proposed by Roberts and Garboczi [11], was considered. In order to keep the periodic conditions of the RVEs, parts of pores or solids that exceeded a face of the RVE was cut and shifted to the opposite face. In the cases of Model A-C, the pores and solids were assumed to be spheres 1 \(\mu\)m in diameter, and 12 \(\times\) 12 \(\times\) 12 \(\mu\)m\(^3\) RVE box was used. For Model D, RVE with a dimension of 10 \(\times\) 10 \(\times\) 10 \(\mu\)m\(^3\) was made up by randomly orientated axi-symmetric oblate ellipsoidal pores with a diameter of 1 \(\mu\)m and a height along rotating axis of 0.25 \(\mu\)m. Details of these geometries as well as size independence of RVE can be found elsewhere (e.g. in ref.[11]), which will not be repeated here. Since this study was mainly focused on the influence of the pore morphology, porosity was fixed to 20% for all models.

Fig. 1. RVEs of pore morphologies used for the simulations. (a) Isolated spherical pores (Model A), (b) Overlapped spherical pores (Model B), (c) Overlapped spherical solids (Model C) and (d) Overlapped ellipsoidal pores (Model D).
Fig. 2. Geometries and meshes of RVE models for porous microstructures. (a) Isolated spherical pores (Model A), (b) Overlapped spherical pores (Model B), (c) Overlapped spherical solids (Model C) and (d) Overlapped ellipsoidal pores (Model D).

3. Effective Elastic and Thermal Properties of the Models

For implementation of the models, a commercial finite element software, ANSYS® [12], was used and porous alumina was chosen for the materials throughout this study to solve the numerical problems. Fig. 2 shows the geometries and meshes of RVE models for porous ceramic microstructures. As shown in the figure, the models were meshed with ten-noded quadratic tetrahedral elements (SOLID187, ANSYS). The finite element meshes were made finer near the pores. The number of elements and node points were approximately 130,000 and 28,000 for Model A and B, 785,000 and 1,164,000 for Model C, and 373,000 and 79,000 for Model D, respectively. The alumina was modeled as linear elastic and thermally isotropic, with density of 3,900 Kg/m$^3$, Poisson’s ratio of 0.25, coefficient of thermal expansion of $8 \times 10^{-6}/\text{°C}$, elastic modulus of 350 GPa, thermal conductivity of 8 W/m·°C and heat capacity of 1,200 J/K·°C.

To predict the effective elastic moduli of the models, three independent uniaxial loads were applied to each model along three coordinate axes. The effective thermal conductivities of the models were also determined from heat flow in three FE simulations using perpendicular temperature gradients and Fourier’s law. The effective elastic moduli, Poisson’s ratios and thermal conductivities for four different RVE models are listed in Table 1, where the statistical variations (equal to twice the standard error) for each parameter are also shown. It was found that both the elastic modulus and thermal conductivity were reduced with a presence of porosity for all cases, as expected. It can be also clearly seen that the elastic and thermal properties of the porous microstructure were markedly influenced by their pore morphologies. The elastic modulus and thermal conductivity of Model C was significantly lower than those of Model A and B, thus indicating that the minimum solid area [13] for overlapped solid spheres is far smaller than that for spherical pores. This can be more clearly seen from values $E/E_{\text{solid}}$ and $\alpha/\alpha_{\text{solid}}$ in Table 1, where $E_{\text{solid}}$ and $\alpha_{\text{solid}}$ are elastic modulus and thermal conductivity for fully dense alumina, respectively: whereas the $E/E_{\text{solid}}$ and $\alpha/\alpha_{\text{solid}}$ for Model C were 0.43 and 0.57, while corresponding values for Model A were 0.68 and 0.73, respectively. Model D shows intermediate levels of elastic modulus and thermal conductivity between other models.

Table 1. Effective elastic and thermal properties of the RVE models.

<table>
<thead>
<tr>
<th></th>
<th>Elastic modulus $(E, \text{ GPa})$</th>
<th>Poisson’s ratio $(\nu)$</th>
<th>Thermal conductivity $(\alpha, \text{ W/m°C})$</th>
<th>$E/E_{\text{solid}}$</th>
<th>$\alpha/\alpha_{\text{solid}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dense alumina</td>
<td>$E_{\text{solid}} = 350$</td>
<td>0.25</td>
<td>$\alpha_{\text{solid}} = 8$</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Model A</td>
<td>$237.5 \pm 3$</td>
<td>0.238</td>
<td>$5.87 \pm 0.04$</td>
<td>0.68</td>
<td>0.73</td>
</tr>
<tr>
<td>Model B</td>
<td>$239.3 \pm 6$</td>
<td>0.235</td>
<td>$5.89 \pm 0.07$</td>
<td>0.68</td>
<td>0.74</td>
</tr>
<tr>
<td>Model C</td>
<td>$150.5 \pm 5$</td>
<td>0.193</td>
<td>$4.54 \pm 0.11$</td>
<td>0.43</td>
<td>0.57</td>
</tr>
<tr>
<td>Model D</td>
<td>$196.4 \pm 21$</td>
<td>0.206</td>
<td>$5.21 \pm 0.40$</td>
<td>0.56</td>
<td>0.65</td>
</tr>
</tbody>
</table>
4. Analysis of Thermal Shock induced Stress

Since the thermally induced stress in ceramic materials relies largely on their elastic and thermal properties when they exposed to the thermal shock, it is worth discussing here the effect of pore morphologies on thermally induced stress in porous ceramics using a specific thermal shock condition with their effective macroscopic material properties. As a test case for this purpose, the numerical simulations of thermal shock test were performed according to ASTM C1525-04 standard by water quenching of heated ceramic rod 10 mm in diameter and 120 mm long [14]. The model and meshes in Fig.3 corresponded to an axi-symmetric 2D representation of the thermal shock test samples. The left body of the mesh corresponded to the axis of symmetry and therefore the heat flows and displacements were fixed in the $z$ direction. Approximately 2,400 three-noded triangular elements (PLANE 182, ANSYS) and 5,000 node points were used. By applying 25 °C water quenching at model boundaries with a film coefficient of 12,000 W/m² for 2 seconds and using initial temperature of 525 °C, thermal stresses were calculated from the temperature distributions of the model.

Fig.4 shows the macroscopic equivalent stress contours for four types of porous microstructures, which were predicted by applying effective elastic and thermal properties of the RVE models (Table 1). Fig.4 also shows the

![Fig. 3. Geometry and meshes of an axisymmetric FE model for ASTM C 1525-04 standard thermal shock test method.](image)

![Fig. 4. Predicted equivalent stress fields after 2 sec water quenching for four types of porous microstructures, showing thermal shock induced stress levels in macroscopic scale. In the figure, corresponding equivalent stress fields in microscopic scale at selected nodes (Node A in Fig.3), are also depicted.](image)
equivalent stress fields in microscopic scale which corresponded to the stress at the selected nodes (Node A in Fig.3), predicted by applying strain components of the node to the RVE models. For all cases, maximum stress occurs near the top surface of the model (near the side surface of the thermal shock specimen). It can be seen that the more stressed nodes in macroscopic scale produced higher level of stress fields in microscopic scale, as expected. There are large differences between stress levels of the models, which are results of the different macroscopic elastic and thermal properties. The level of stress was significantly higher in Model A and B than that in Model C, indicating that the level of thermally induced stress in this test condition is dominated by the elastic modulus rather than the thermal conductivity. This may be due to the high elastic moduli of Model A and B, compared to that of Model C.

The numerical results presented here is valuable to discuss the effect of pore morphology on the thermal shock resistance of some ceramic materials. When interpreting the numerical results in Fig.4, the effect of inter-connection between pores on the thermal shock induced stress is likely negligible since the difference in stress level between Model A and B is not significant. For given porosity and in case of rapid cooling, relatively weak structure (e.g. partially sintered structure such as overlapped solid spheres, Model C) is advantageous to prevent thermal shock damage than stiffer microstructure. Ellipsoidal pores tend to reduce overall stiffness more than spherical pores, thus a material having oblate-like pores seems more desirable for this particular condition than having spherical pores.

5. Conclusions

In this paper, the influence of the pore morphology on the thermal shock characteristics of the porous ceramic materials was investigated using finite element simulations of four different porous microstructures. Through the numerical analyses, it was shown that the thermal shock characteristics of the porous materials were strongly related to their pore morphology.

The inter-connection between pores did not alter much the thermal shock induced stress. In contrast, changes in pore shape from spherical to ellipsoidal markedly reduced the level of thermal stress. For porosity of 20% and in case of rapid water quenching, it is likely that the level of thermally induced stress is mainly determined by the elastic modulus of the microstructure. In this particular situation, relatively weak microstructure such as partially sintered ceramics seems to be advantageous to prevent thermal shock damage and fracture.

The numerical results presented here suggest that consideration of pore morphology can give qualitative information on the thermal shock characteristics of the materials, and thus may helpful to design and optimize porous ceramics.

References