Constitutional Dependence of Thermal Conductivity in Dispersion Composites*

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The thermal conductivity of Mo fiber-reinforced Al₂O₃ composite was calculated using analytical solutions for effective thermal conductivity. The deviation between calculated and literature data was less than 10%. The influence of constitution on thermal conductivity of dispersion composites was investigated by simulation based on analytical solutions. When the reinforcements are unidirectionally arrayed, their volume, shape and thermal conductivity greatly affects the thermal conductivity of the composite, and the effects on the thermal conductivity parallel to the reinforcement orientation are bigger than those on the thermal conductivity along the perpendicular direction. As the orientation of reinforcements becomes increasingly random, the anisotropy of thermal conductivity becomes smaller and smaller.

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1. Introduction

Theoretical and experimental research has revealed that the effective thermal conductivity of a composite depends on its component materials and structure. Therefore, it is possible to select a specific thermal conductivity for a composite by choosing appropriate materials and designing its structure. For this purpose, a study of the dependencies of thermal conductivity on these constitutional factors is needed.

In our previous work,¹ we developed an analytical solution-based thermal conductivity calculation engine, in which are included analytical solutions for thermal conductivity that have so far been derived with various composite models. The constitution of a composite is described by a file written in Extensible Markup Language (XML), which can be easily edited using a text editor or automatically generated by a computer. The engine analyzes the file, recognizes the composite model, and selects the optimal analytical solution for calculating its thermal conductivity. Because of its ease of constitutional design and fast calculation speed, it is ideal for studying patterns of change in thermal conductivity while adjusting the levels of various constitutional parameters.

In this study, the accuracy of calculation is evaluated by comparison with data in the literature; the dependencies of thermal conductivity on various constitutional parameters were then investigated for dispersion composites.

2. Accuracy of Calculation

Literature data of thermal conductivity of a Mo fiber-reinforced Al₂O₃ composite² is used as a reference for evaluating the accuracy of calculation. The composite is reported to be prepared from alumina of grain size 5–9 μm and non-annealed Mo short fiber. The batches were thoroughly mixed, charged into a graphite mold, hot pressed at 1650°C at 2.07 x 10⁷ Pa and cooled to room temperature in about 4 hours. The mass percentage is 90% for Al₂O₃ and 10% for Mo. With densities of 10240 kg/m³ for Mo³ and 4000 kg/m³ for Al₂O₃,⁴ the fiber volume fraction is calculated to be 0.043. The geometry of the fibers is described as a cylinder 0.051 mm in radius and 3.175 mm in length. All fibers are arrayed along the direction of the x₁ axis. k₁, k₂ and k₃ are thermal conductivities along the x₁, x₂ and x₃ axes, respectively.

Table 1 Comparison of literature and calculated thermal conductivity of Mo-reinforced Al₂O₃ composite.

<table>
<thead>
<tr>
<th>T (K)</th>
<th>k₁ (Wm⁻¹K⁻¹)</th>
<th>k₂ (Wm⁻¹K⁻¹)</th>
<th>k₃ (Wm⁻¹K⁻¹)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Experimental</td>
<td>Calculated</td>
<td>Experimental</td>
</tr>
<tr>
<td>366.5</td>
<td>31.8</td>
<td>30.95</td>
<td>33.1</td>
</tr>
<tr>
<td>477.6</td>
<td>24.9</td>
<td>22.96</td>
<td>26.2</td>
</tr>
<tr>
<td>588.7</td>
<td>19.5</td>
<td>17.42</td>
<td>20.7</td>
</tr>
<tr>
<td>699.8</td>
<td>15.1</td>
<td>13.52</td>
<td>16.1</td>
</tr>
<tr>
<td>810.9</td>
<td>12.11</td>
<td>11.00</td>
<td>13.2</td>
</tr>
<tr>
<td>913.7</td>
<td>10.9</td>
<td>9.43</td>
<td>11.5</td>
</tr>
<tr>
<td>Average deviation</td>
<td>9.0%</td>
<td>6.7%</td>
<td></td>
</tr>
</tbody>
</table>

Fig. 1 Structural model of the Mo-reinforced Al₂O₃ composite. Mo fibers are arrayed along the x₁ axis. k₁, k₂ and k₃ are thermal conductivities along the x₁, x₂ and x₃ axes, respectively.

Table 1

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shows that the calculated thermal conductivities deviate from the experimental results at an average of 9.0% for \( k_1 \) and 6.7% for \( k_3 \).

3. Dependence of Thermal Conductivity on Constitu-

tional Parameters

In a review\(^1\) of theories on thermal conductivity, we have concluded that the effective thermal conductivity of a dispersion composite depends on the thermal conductivity of the matrix, the thermal conductivity of dispersion, and the volume fraction, geometry and orientation of dispersion. In the present study, the interfacial thermal resistance between matrix and dispersion has been neglected.

3.1 Effect of constitutional state

The influences of fiber volume fraction, shape and orientation on thermal conductivity were separately investigated for the above Mo–Al\(_2\)O\(_3\) composite.

The thermal conductivities calculated with different fiber volume fractions are shown in Fig. 2(a). Both \( k_1 \) and \( k_3 \) increase with increasing volume fraction. \( k_3 \), the thermal conductivity in the direction parallel to the fibers, increases faster than \( k_1 \), which is perpendicular to the fibers.

The geometry of a fiber can be approximately described by an ellipsoid with semi axes \( a \) and \( c \). When \( c \) tends to infinity (\( a/c = 0 \)), it represents a cylinder; \( a/c < 1 \), a prolate spheroid; \( a/c = 1 \), a sphere; and \( a/c > 1 \), an oblate spheroid. The thermal conductivities with fiber shapes of cylinder, sphere and oblate spheroid are calculated for the Mo–Al\(_2\)O\(_3\) composite and shown in Fig. 2(b). When fiber shape changes from cylinder to sphere (\( a/c \) increases from 0 to 1), \( k_3 \) decreases, whereas \( k_1 \) increases slightly. When fiber shape changes from sphere to oblate spheroid (\( a/c \) increases from 1 to 100), there is a slight decrease observed in \( k_3 \), while \( k_1 \) markedly increases. The responses of \( k_3 \) and \( k_1 \) to the change of fiber shape are opposed.

All fibers in the above composite were arrayed along the \( x_3 \) axis (1-dimensional orientation). If the orientation of the fiber changes, the thermal conductivity changes as well. The orientation of fiber is described by two angles \( \alpha \) and \( \varphi \) as shown in Fig. 3. If the axes of all fibers are located in the \( x_1-x_3 \) plane (\( \varphi = 0 \)), and the fiber orientation with respect to \( \alpha \) is completely random, the result is 2-dimensional random orientation. Similarly, when the fiber orientation with respect to both \( \alpha \) and \( \varphi \) is random, the result is 3-dimensional random orientation. The thermal conductivities for 1-dimensional (1D), 2-dimensional (2D) random and 3-dimensional (3D) random orientation are calculated and shown in Table 2. The fiber volume fraction is assumed in the calculations to be 0.1. Maximum anisotropy of thermal conductivity is observed when fibers take a 1-dimensional orientation. As fiber orientation becomes increasingly random, the difference of

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**Table 2** Thermal conductivities of the Mo-reinforced Al\(_2\)O\(_3\) composite with 1-dimensional, 2-dimensional random and 3-dimensional random fiber orientations.

<table>
<thead>
<tr>
<th></th>
<th>1D distribution</th>
<th>2D random distribution</th>
<th>3D random distribution</th>
</tr>
</thead>
<tbody>
<tr>
<td>( k_1 )</td>
<td>(Wm(^{-1})K(^{-1}))</td>
<td>(Wm(^{-1})K(^{-1}))</td>
<td>(Wm(^{-1})K(^{-1}))</td>
</tr>
<tr>
<td>( k_2 )</td>
<td>19.04</td>
<td>19.04</td>
<td>19.04</td>
</tr>
<tr>
<td>( k_3 )</td>
<td>27.62</td>
<td>23.47</td>
<td>22.03</td>
</tr>
</tbody>
</table>

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Fig. 2 Thermal conductivities of the Mo-reinforced Al\(_2\)O\(_3\) composite with different fiber volume fractions (a) and different fiber shapes (b).

Fig. 3 Description of fiber orientation.
thermal conductivity in different directions becomes smaller and smaller. Finally, when the composite shows 3-dimensional random orientation, thermal conductivity becomes isotropic.

### 3.2 Effect of dispersion of reinforcements

The dependence of thermal conductivity on the thermal conductivities of reinforcements and matrix and on reinforcement shape is shown in Fig. 4. The reinforcements are assumed to be unidirectionally arrayed along the \( x_3 \) axis, and the volume fraction is assumed to be 0.4. \( k_3 \) is the thermal conductivity in the direction parallel to reinforcements, and \( k_1 \) perpendicular to it. \( k_d \) and \( k_m \) are the thermal conductivities of reinforcements and matrix, respectively, and both are assumed to be isotropic. \( a \) and \( c \) are semi-axes of ellipsoidal reinforcements. Figure 4 shows that the reinforcement shape and thermal conductivity of reinforcements and matrix greatly affect the thermal conductivity of the composite. Generally, the effect on \( k_3 \) is much greater than that on \( k_1 \).

The reinforcement shape in Fig. 4 may be divided into three regions:

1. \( \log(c/a) < 0 \). When the reinforcements take the shape of oblate spheroids, the changes in shape and thermal conductivity have little influence on \( k_3 \), while that on \( k_1 \) is marked. \( k_1 \) decreases with increasing \( c/a \), and increases with increasing \( k_d/k_m \).

2. \( 0 \leq \log(c/a) < 2 \). When the reinforcements are in the shape of spheres or prolate spheroids, the influences of shape and thermal conductivity on \( k_3 \) become marked. \( k_3 \) increases sharply with increasing \( c/a \) and \( k_d/k_m \). The influence of shape on \( k_1 \) becomes insignificant. \( k_1 \) increases with increasing \( k_d/k_m \) until \( k_d/k_m = 20 \), and then levels off.

3. \( \log(c/a) \geq 2 \). When reinforcements are in a shape approximating a cylinder, any change in \( c/a \) will have little influence on \( k_3 \) or \( k_1 \). With increasing \( k_d/k_m \), \( k_3 \) increases linearly, while, as in (2), \( k_1 \) increases up to \( k_d/k_m = 20 \), then remains stable.

Figure 5 shows the dependence of thermal conductivity on volume fraction and orientation of reinforcements. The reinforcements are assumed to be cylindrical, and \( k_d/k_m \) is assumed to be 20. The orientation of reinforcements is described in the same way as Fig. 3. Orientation with respect to \( \phi \) is completely random. The distribution of \( \alpha \) is assumed to be uniform between \( -\alpha_{max} \leq \alpha \leq \alpha_{max} \) and 0 beyond that. Thermal conductivity has been calculated with the volume fraction and orientation of reinforcements.
fraction changing from 0 to 0.5 and $\alpha_{\text{max}}$ from 0 to $\pi/2$. The thermal conductivity increases with increasing volume fraction. As the orientation of reinforcements becomes increasingly random, the increase in $k_3$ slows down and the increase in $k_1$ accelerates.

4. Conclusion

The thermal conductivity of Mo fiber-reinforced Al$_2$O$_3$ composite was calculated using analytical solutions for effective thermal conductivity for composites. By comparing the results to data in the literature, the accuracy of calculation was evaluated as being within 10%. Then, by changing the structural parameters of the composite one by one, the dependencies of thermal conductivity on constitutional conditions were investigated. Finally, relationships between thermal conductivity and constitution of dispersion composites were obtained. These results are expected to be helpful in designing composites with specific thermal conductivities.

REFERENCES