Heat Conduction in Ceramic Coatings: Relationship between Microstructure and Effective Thermal Conductivity

Technical report for Task 2 (Second Year)

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Analysis of the effective thermal conductivity of ceramic coatings and its relation to the microstructure continued. Results (obtained in Task 1) for the three-dimensional problem of heat conduction in a solid containing an inclusion (or, in particular, cavity - thermal insulator) of the ellipsoidal shape, were further advanced in the following two directions:

- closed form expressions of $H$ tensor have been derived for special cases of ellipsoidal cavity geometry: spheroid, crack-like spheroidal cavity and needle shaped spheroidal cavity;
- these results for one cavity have been incorporated to contrast heat energy potential for a solid with many spheroidal cavities (in the approximation of non-interacting defects).

This problem constitutes a basic building block for further analyses, since the ellipsoidal shape covers a variety of practically important pore geometries.

The problem is formulated as the determination of the change in thermal conductivity due to inclusion. Namely:

$$\Delta Q = H \cdot G$$  (1)
where $\Delta Q$ is the heat flux change per reference volume $V$, $G$ is the far-field temperature gradient and second rank tensor $H$ is a function of the inclusion shape and the inclusion conductivity.

Mathematical considerations based on the analysis of the ellipsoidal shapes in the framework of Eshelby-type theory and on utilization of Green's function for the heat conduction problem in an unbounded medium, show that $H$ has the following form:

$$H = \frac{V^*}{V} (k* - k_0) (A_1 ll + A_2 mm + A_3 nn)$$

(2)

where $V^* = \frac{4\pi}{3}a_1a_2a_3$ is the volume of the ellipsoidal inclusion with semi-axes $a_1, a_2, a_3$ with unit vectors $l, m, n$; $k*$ and $k_0$ are conductivities of the inclusion and of the matrix, correspondingly. Coefficients $A_1, A_2, A_3$ are given in terms of elliptic integrals (see Report for Task 1).

In the case when the inclusion is a spheroid ($a_1 = a_2 = a$), tensor $H$ takes the form

$$H = \frac{V^*}{V} (k* - k_0) \left\{ 1 + \frac{k* - k_0}{k_0} f_0(\gamma) \right\}^{-1} (I - nn) + \left\{ 1 + \frac{k* - k_0}{k_0} (1 - 2f_0(\gamma)) \right\}^{-1} nn$$

(3)

or, in components:

$$H_{ij} = \frac{V^*}{V} (k* - k_0) \left\{ 1 + \frac{k* - k_0}{k_0} f_0(\gamma) \right\}^{-1} (\delta_{ij} - n_i n_j) + \left\{ 1 + \frac{k* - k_0}{k_0} (1 - 2f_0(\gamma)) \right\}^{-1} n_i n_j$$

(4)

where it is denoted:

- $\gamma = a/a_3$ - aspect ratio of the spheroidal inclusion,
- $n = n_1e_1 + n_2e_2 + n_3e_3$ - unit vector along the axis of symmetry of spheroid,
- $I = e_1e_1 + e_2e_2 + e_3e_3$ - unit second rank tensor,
- $f_0(\gamma) = \frac{1 - g(\gamma)}{2(1 - \gamma^2)}$, $g(\gamma) = \frac{\gamma^2}{\sqrt{\gamma^2 - 1}} \arctan\sqrt{\gamma^2 - 1}$ (for oblate shape, $\gamma > 1$),
- $g(\gamma) = \frac{\gamma^2}{2\sqrt{1 - \gamma^2}} \ln\frac{1 + \sqrt{1 - \gamma^2}}{1 - \sqrt{1 - \gamma^2}}$ (for prolate shape, $\gamma < 1$).
• In the case of spheroidal cavity (insulator, \( k_s = 0 \)) tensor \( H \) is as follows:

\[
H = -\frac{V^*}{V} k_0 \left\{ \frac{1}{1 + f_0(y)} (I - nn) + \frac{1}{2f_0(y)} nn \right\}
\]  

(5)

• In the case of thin spheroidal cavity (\( \gamma \gg 1 \)):

\[
H = -\frac{V^*}{V} k_0 \left\{ \frac{1}{1 + \pi/(4\gamma)} (I - nn) + \frac{2\gamma}{\pi} nn \right\}
\]

(6)

• In the limit of a circular crack:

\[
H = -\frac{8a^2}{3V} k_0 nn
\]

(7)

• In the case of needle-shaped spheroidal cavity (\( \gamma \ll 1 \)):

\[
H = -\frac{V^*}{V} k_0 \left\{ \left[ 1 - \frac{1}{2} \left( 1 + \gamma^2 - \gamma^2 \ln \frac{2}{\gamma} \right) \right]^{-1} (I - nn) + \left( 1 + \gamma^2 - \gamma^2 \ln \frac{2}{\gamma} \right) nn \right\}
\]

(8)

In the approximation of non-interacting cavities (each cavity experiences the influence of the same far-field temperature gradient \( G \) unperturbed by the presence of other cavities), the heat energy potential \( \Delta \Omega \) for a solid with many cavities is obtained as follows (in terms of derived tensors \( H^{(i)} \) characterizing \( i \)-th cavity):

\[
\Delta \Omega = \frac{1}{2} G \cdot \left[ \sum_i H^{(i)} \right] \cdot G
\]

(9)

For example, in the case of spherical cavities we have:

\[
\sum_i H^{(i)} = -\frac{3}{2} k_0 I \left[ \frac{1}{V} \sum_i V^{(i)} \right] = -\frac{3}{2} pk_0 I
\]

(10)

\[
\Delta \Omega = -\frac{3}{4} pk_0 G \cdot G = -\frac{3}{4} pk_0 \left( G_1^2 + G_2^2 + G_3^2 \right)
\]

(10a)
where parameter $p$ is the conventional porosity.

In the case of circular cracks we have:

$$\sum_{i} H^{(i)} = -\frac{8}{3} k_0 \left[ \frac{1}{V} \sum (a^3 n n)^{(i)} \right] = -\frac{8}{3} k_0 a$$

(11)

$$\Delta \Omega = -\frac{4}{3} k_0 G \cdot a \cdot G$$

(11a)

where $a$ is the second rank crack density tensor (well known in problems of effective elastic properties of cracked media).
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