Explicit relations between elastic and conductive properties of materials containing annular cracks

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Published online 26 March 2003

The impact of annular cracks on the effective elastic and conductive properties of a material is analysed. The compliance contribution tensor of an annular crack—the quantity that determines the increase in compliance of a solid due to introduction of such a crack—is derived analytically. The resistivity contribution tensor of an annular crack is calculated numerically. It is shown that an effective circular crack, i.e. a crack which yields the same change in elastic/conductive properties of a material as the given annular crack, can be chosen to match both of these tensors. Using this result, the explicit relation between elastic and conductive properties of a material containing annular cracks is obtained. The relation is derived using a non-interaction approximation. Applicability of the derived formulae to real materials (to plasma-sprayed coatings, in particular) is discussed.

Keywords: annular cracks; cross-property relations; plasma-sprayed coatings

1. Introduction

Cross-property correlations constitute one of the most challenging problems of materials science and have been examined by several authors in the past. Aside from early work by Bristow (1960) on the conductivity–elasticity relation for a material with a low concentration of randomly oriented microcracks, and by Levin (1967) on the connection between the bulk modulus and the thermal-expansion coefficient of a two-phase isotropic composite, most of the analyses have been focused on constructing bounds for the cross-property correlations. Such bounds were investigated in the work of Berryman & Milton (1988) on two-phase isotropic composites. They were substantially advanced by Gibiansky & Torquato (1995, 1996a, b), who narrowed them, under additional restrictions on the composite microgeometry and on the properties of constituents. The mathematical aspects of cross-property correlations were thoroughly discussed by Milton (1997) and Markov (1999).

The practical needs of materials science call, however, for cross-property correlations that, preferably,

(i) have an explicit form;

(ii) can be applied to strongly anisotropic microstructures (such as coatings, reinforced plastics, etc.); and

One contribution of 12 to a Theme ‘Micromechanics of fluid suspensions and solid composites’.
Figure 1. Microstructure of a sprayed coating contains splats with imperfect bonds between the horizontal interfaces and vertical cracks and pores inside the splats. (a) Microphotograph of yttrium-stabilized zirconia coating; (b) micromechanical model.

(iii) remain accurate when there is a high contrast between the phases (materials with pores, microcracks or hard particles).

Correlations of this kind were recently obtained by Sevostianov & Kachanov (2001, 2002) and Kachanov et al. (2001) for materials containing spheroidal inclusions or pores. They explicitly interrelated full sets of anisotropic elastic and conductive constants of heterogeneous materials that contain inhomogeneities such as spheroidal shapes and orientations.

The cross-property correlation is derived in the framework of a non-interaction approximation. In the cases when the interactions between inhomogeneities cannot be neglected, the hypothesis of Bristow—that the interactions affect both groups of properties (elastic and conductive) in a similar way (so that the cross-property correlations continue to hold, although this approximation may yield substantial errors for each of the properties separately)—was verified experimentally by Sevostianov et al. (2002) for porous materials, and by Bogarapu & Sevostianov (2002) for microcracked materials.

Note that the results derived by Kachanov et al. (2001) and Sevostianov & Kachanov (2001, 2002) are limited to spheroidal shapes, when Eshelby’s theorem (Eshelby 1957, 1961) is applicable. In this paper, we analyse material containing annular cracks that cannot be described using such a technique.

A typical example of a material containing annular cracks is plasma-sprayed coating. At the present stage, coatings are modelled as having a lamellar microstructure consisting of elongated, flat-like splats with diameters of the order of 100–200 μm and thicknesses of 2–10 μm, formed by a rapid solidification (figure 1). Although the porous space comprises micropores and microcracks of diverse shapes and orienta-
tions, overall, it has a highly anisotropic structure. This results in anisotropic elastic stiffnesses and thermal conductivities.

In order to explicitly express the effective properties in terms of the microstructural parameters, the complexity of the porous space has to be reduced to several dominant elements. Usually, the dominant elements of the porous space are identified as two families of strongly oblate pores (circular cracks) that tend to be approximately parallel and approximately perpendicular to the substrate (Leigh & Berndt 1999; Sevostianov & Kachanov 2000).

An important observation is that the attempts to evaluate the effective elastic moduli of the coating, based on those values of the crack density that are recovered from microphotographs, tend to strongly disagree with the available experimental data (up to one order of magnitude). The values of the crack density were recovered from microphotographs under the assumption that line cracks in two-dimensional cross-sections represent traces of isolated, circular, three-dimensional cracks.

This led us to the conclusion that the mentioned assumption should be re-examined. According to the concepts suggested by Kudinov (1977) and schematically presented in figure 2, the areas of cohesion alternate with no-contact areas. Therefore, the line cracks that are visible in the two-dimensional cross-sections are

Figure 2. Schematic of splat formation (deformation of a particle due to a stroke against a plane surface): (a) initial state; (b) final state.
likely to represent an annular (rather than circular) type of crack. Thus, in order to model the presence of ‘islands’ of cohesion that alternate with areas of no cohesion, we need to introduce annular cracks as essential microstructural elements.

In this paper, we suggest a method for the calculation of the compliance contribution tensor of an annular crack and show how the effective circular crack may be chosen (a circular crack, which yields the same change in elastic properties as the given annular crack). The conductivity problem is then solved numerically and the effective circular crack is also obtained. We find that it almost coincides with those for the elasticity problem (agreement is better than 3%). This fact allows us to expand the cross-property correlation to the case of a material containing annular cracks.

2. Effective elastic properties of material containing circular cracks

We briefly summarize the results on the effective elasticity of materials with pores of diverse shapes and orientations that are relevant for our analyses (see Kachanov et al. (2001) and Sevostianov & Kachanov (2002) for details).

For a solid of volume $V$ containing one cavity (of volume $V_{\text{cav}}$), the total strain per $V$ under remotely applied stress tensor $\sigma$ can be represented as a sum:

$$\varepsilon_{ij} = S_{ijkl}^0 \sigma_{kl} + \Delta \varepsilon_{ij}, \quad (2.1)$$

where $S_{ijkl}^0$ is the compliance tensor of the matrix and $\Delta \varepsilon_{ij}$ is the extra strain due to the cavity. Due to linear elasticity, $\Delta \varepsilon_{ij}$ is a linear function of the applied stress:

$$\Delta \varepsilon_{ij} = H_{ijkl}^E \sigma_{kl}, \quad (2.2)$$

where $H_{ijkl}^E$ is the fourth-rank cavity compliance tensor (the superscript ‘E’ stands for elasticity here, in contrast with the superscript ‘C’ below, which stands for conductivity).

Tensor $H_{ijkl}^E$ was calculated for the ellipsoidal shapes by Kachanov et al. (1994) (see also Kanaun 1983). It has been shown that (Kachanov et al. 2001; Sevostianov & Kachanov 2002), for the spheroidal pore (semi-axes $a_1 = a_2 \equiv a$, aspect ratio $\gamma = a_3/a < 1$ and $n_i$ is a unit vector along the spheroid’s axis of symmetry), $H_{ijkl}^E$ can be approximated by the following expression:

$$H_{ijkl}^E \approx \frac{1}{E_0} \frac{V_{\text{cav}}}{V} [B_1 \delta_{ij} \delta_{kl} + B_2 J_{ijkl} + B_3 (n_i n_s J_{sijkl} + J_{ijksn_sn_l}) + B_4 (n_i n_j \delta_{kl} + \delta_{ij} n_k n_l)], \quad (2.3)$$

where coefficients $B_i$ depend on the aspect ratio $\gamma$ and on Poisson’s ratio of the solid phase $\nu_0$, and where $J_{ijkl} = (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk})/2$. The important simplification in (2.3) is that, in contrast with the exact form of $H_{ijkl}^E$, the approximation (2.3) contains quadratic terms $n_i n_j$, but not fourth-order terms $n_i n_j n_k n_l$.

Note that, with the trivial exception of a sphere, the representation (2.3) does not hold exactly, but is satisfied, with good accuracy, for spheroids. The error depends on the spheroid’s aspect ratio and on Poisson’s ratio $\nu_0$ of the matrix. Being zero for a sphere, the error increases for shapes that are either increasingly oblate or increasingly prolate, reaching 8% and 4% (for $\nu_0 = 0.3$) in the limits of a crack and a cylinder, respectively. As far as the dependence on $\nu_0$ is concerned, the error decreases for smaller $\nu_0$ (and becomes negligibly small for all shapes at $\nu_0 < 0.15$).
The significance of the approximation (2.3) is that, for a solid with many pores, summation over tensors \( H_{ijkl}^E \) will give rise to a second- (rather than fourth-) rank tensor, characterizing the pore distribution. This approximation has far-reaching implications: besides simplifications in the overall elastic anisotropy, it leads to correlations between the elastic and the conductive properties.

In the limit of a circular crack, the expression for \( H_{ijkl}^E \) is reduced to

\[
H_{ijkl}^E = \frac{16(1 - \nu_0^2)}{3(2 - \nu_0)E_0} \frac{a^3}{V} \left( n_in_sn_sJ_{sijkl} + J_{ijkl}n_sn_n \right).
\]

The important observation given by Kachanov et al. (2001) is that the expression (2.4) for the crack can actually be used for the strongly oblate pores (aspect ratio \( \gamma < 0.15 \)). This means that the strongly oblate pores can be replaced by cracks, as far as their contribution to the overall compliances is concerned. This further implies that the proper parameter, in terms of which the effective compliances are to be expressed, is the crack density, with porosity \( p \) (volume fraction of pores) playing a secondary role.

For a solid with many pores, the individual (\( m^{th} \)) pore contributions \( \Delta \varepsilon_{ij}^{(m)} \) to the overall strain are to be summed over the set of pores. In the simplest approximation of non-interacting pores (each pore is subjected to the same stress \( \sigma_{ij} \), unperturbed by the neighbours), the extra strain due to the presence of pores is

\[
\Delta \varepsilon_{ij} = \sum_m (\Delta \varepsilon_{ij}^{(m)}) = \left( \sum_m (H_{ijkl}^E)^{(m)} \right) \sigma_{kl},
\]

where the individual \( (H_{ijkl}^E)^{(m)} \) tensors are given by (2.3).

For cracks,

\[
\sum_m (H_{ijkl}^E)^{(m)} = \frac{16(1 - \nu_0^2)}{3(2 - \nu_0)E_0} \left[ \alpha_{is}J_{sijkl} + J_{ijkl}\alpha_{sl} \right],
\]

and the overall compliances are expressed in terms of the symmetric second-rank crack-density tensor

\[
\alpha_{ij} = \frac{1}{V} \sum_m (a^3n_in_j)^{(m)},
\]

where \( a^{(m)} \) is the \( m^{th} \) crack radius. Note that its trace

\[
\rho = \alpha_{ii} = \frac{1}{V} \sum_m a^{(m)3}
\]

is the usual crack-density parameter. As discussed above, expression (2.6) applies not only to cracks, but also to pores of strongly oblate shapes (up to aspect ratios \( \gamma < 0.15 \)).

3. Elastic compliance of an annular crack

We consider an annular crack bounded by two concentric circles, of radii \( a \) and \( a - c \) (Figure 3), and estimate normal compliance \( B_{nn} \) of the crack by

(i) using the general relation between the elastic compliances of cracked solids and stress intensity factors (SIFs) along crack edges; and

(ii) using the available result for the SIF at the outer edge of the annular crack.

\[\text{Phil. Trans. R. Soc. Lond. A (2003)}\]
The SIFs at the outer and inner edges of the annular crack were calculated by Smetanin (1968) with the asymptotic method, and by Moss & Kobayashi (1971) with the integral transform method (method of Mossakovsky and Rybka (see Mossakovsky 1955)). The accuracy of the results is 1% for the SIF at the outer edge and 2% for the SIF at the inner edge (Rooke & Cartwright 1976). The results are given in the form

$$K_I = \frac{\sigma_{33}}{2 \pi} \sqrt{\frac{a}{c}} F(\lambda), \quad (3.1)$$

where $\lambda = c/a$ and functions $F(\lambda)$ for inner and outer edges are presented in figure 3. Note that this function at the outer edge can be approximated as a linear one with the accuracy better than 3% (for the inner edge the accuracy of linear approximation is about 6%). Then the SIF at the outer edge of the annular crack can be approximated by the following expression:

$$K_I = \frac{\sigma_{33}}{2 \pi} \sqrt{\frac{a}{c}} \sqrt{\frac{2 \sqrt{2}}{\pi}} \lambda (\sqrt{\frac{2 \sqrt{2}}{\pi}} \lambda + 1 - \lambda). \quad (3.2)$$

We now use the general relation between SIFs and the effect of cracks on the overall elastic compliances derived by Rice (1975). For a reference volume $V$ containing one or several cracks that may propagate, the increment $dS_{ijkl}$ of the overall compliance due to incremental advance $dl$ on all propagating crack fronts, collectively denoted by $L$, can be represented in the form

$$dS_{ijkl} = \frac{1 \, \frac{1}{4}}{V} \int_L \left( c_{qr} \frac{\partial K_q}{\partial \sigma_{ij}} \frac{\partial K_r}{\partial \sigma_{kl}} \right) dl, \quad (3.3)$$

where the coefficients $c_{qr}$ relate the near-tip displacement discontinuity to the SIFs:

$$[u_i] = c_{ij} K_j \sqrt{r/2\pi}. \quad (3.4)$$

In the case of the isotropic matrix, there is no coupling between mode I and modes II and III, so that, for the normal displacement discontinuity $[u_3]$, the only relevant
Figure 4. (a) Compliance of the annular crack as a function of the relative area of the island; (b) radius of the equivalent circular crack in dependence on \( \lambda \) at various values of the Poisson ratio of the matrix.

The compliance coefficient is \( c_{31} \); for the (locally) plane-strain conditions, \( c_{31} = 8(1 - \nu_0^2)/E_0 \). Since \( K_I \) depends only on component \( \sigma_{33} \) of the applied stress, we have

\[
\frac{dS_{3333}}{V} = \frac{1}{E_0} \left( \frac{2(1 - \nu_0^2)}{E_0} \right) \int_L \left[ \left( \frac{\partial K_1}{\partial \sigma_{33}} \right)^2 dl \right] dL,
\]  

and, since \( n = e_3 \), we have \( dS_{3333} = (1/V)B_{nn} \). In our case of the annular crack, we treat this crack as having grown from an infinitesimally thin circular line outwards (with a circular ‘island’ remaining in the final configuration). Then \( L \) is the crack’s outer edge and the integrand is a purely geometrical factor obtained from (3.2).

Hence, calculation of the compliance change due to a certain amount of crack growth, and of the normal crack compliance \( B_{nn} \), reduces to integration of the mentioned factor over the area of the advance:

\[
B_{nn} = \frac{1}{V} \frac{2\pi(1 - \nu_0^2)}{E_0} a^3 \left[ -\lambda^3 \left( \frac{2\sqrt{2}}{\pi} - 1 \right)^2 \ln(1 - \lambda) + \frac{1}{2}(\lambda^2)(2 - \lambda) + 2\lambda^3 \left( \frac{2\sqrt{2}}{\pi} - 1 \right) \right].
\]

Figure 4a gives the radius \( R_{eff} \) of the ‘equivalent’ circular crack that has the same normal compliance \( B_{nn} \) as the annular crack at various values of the Poisson ratio of the matrix; figure 4b shows \( B_{nn} \) in terms of the relative area of the ‘island’.

In the limit of \( \lambda \ll 1 \) (narrow ring), we have approximately plane-strain conditions and \( B_{nn} = 2\pi ac^2(1 - \nu^2)/E \) as expected (multiplier \( 2\pi a \) represents the length of the ring). In the limit of \( \lambda \to 1 \), \( B_{nn} \), formally speaking, should approach \( 16(1 - \nu^2)a^3/3E \), its value for the circular crack of radius \( a \). Formula (3.5) does not yield this limiting value; moreover, the logarithmic term tends to infinity in this limit (although, even at \( 1 - \lambda = 10^{-20} \), \( B_{nn} \), as given by (3.5), still remains lower than \( B_{nn} \) for the circular crack). This is due to the fact that \( K_I \), as given by (3.1), is an approximation of numerical results that may have up to 3% error.

We now illustrate the implications of the effect of a cohesion ‘island’ (modelled by an annular crack) with a simple example; the interpretation of two-dimensional cross-sectional information is shown schematically in figure 5. There are a number of
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Figure 5. Two possible three-dimensional interpretations of two-dimensional pictures: two circular cracks of radius $a/4$, and one annular crack with inner radius $a/2$ and outer radius $a$.

three-dimensional interpretations of this figure. Let us compare two of them: (i) cross-sections of two circular cracks; and (ii) the cross-section of an annular crack.

In the first case, there are two circular cracks of radius $a/4$ and the third component of the crack-density tensor is

$$
\alpha_{33} = \frac{2}{V} \left( \frac{1}{4} a \right)^3 = 0.03125 a^3.
$$

(3.7)

In the second case, we have an annular crack with outer radius $a$ and inner radius $c$. According to figure 3a, the radius of the effective circular crack is $0.6a$ and the third component of the crack-density tensor is

$$
\alpha_{33} = \frac{(0.522a)^3}{V} = 0.143 a^3.
$$

(3.8)

Since the elastic moduli are proportional to the components of the crack-density tensor, the difference in the moduli, calculated according to these two interpretations, is 4.6 times. Thus, the difference between elastic properties, calculated according to these two interpretations, is quite substantial, and some additional information (besides two-dimensional images) is required for calculation of the effective properties.

4. Conductivity of a microcracked solid

We consider a reference volume $V$ of a material, with isotropic thermal conductivity $k_0$, that contains a cavity. The cavity will be modelled as an ideal insulator (although the analysis can be modified, in a straightforward way, to account for the finite conductivity of a pore filled with, for example, a conducting gas). The change in temperature gradient $\Delta G$ (per volume $V$) due to the cavity is a linear function of the far-field heat-flux vector $Q^0$ and hence can be written in the form:

$$
\Delta G = H^R \cdot Q^0,
$$

(4.1)
Table 1. Relative effective resistivity change in dependence on $\lambda = c/a$ calculated with PDEase®

<table>
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<tr>
<th>$c/a$</th>
<th>1.00</th>
<th>0.98</th>
<th>0.96</th>
<th>0.94</th>
<th>0.92</th>
<th>0.90</th>
<th>0.80</th>
<th>0.70</th>
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<tr>
<td>$\frac{k_0 - k_3}{a^3 k_0 k_3}$</td>
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<td>0.1042</td>
<td>0.1026</td>
<td>0.0996</td>
<td>0.0947</td>
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<td>0.0641</td>
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<table>
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<tr>
<th>$c/a$</th>
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<th>0.40</th>
<th>0.30</th>
<th>0.20</th>
<th>0.10</th>
<th>0.08</th>
<th>0.06</th>
<th>0.04</th>
<th>0.02</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\frac{k_0 - k_3}{a^3 k_0 k_3}$</td>
<td>0.0360</td>
<td>0.0242</td>
<td>0.0142</td>
<td>0.0066</td>
<td>0.0018</td>
<td>0.0012</td>
<td>0.0007</td>
<td>0.0003</td>
<td>0.0001</td>
</tr>
</tbody>
</table>

where the second-rank tensor $H^R_{ij}$ is the resistivity contribution tensor of a pore (the superscript ‘R’ stands for resistivity). It is a function of the pore shape. For the spheroidal cavity,

$$H^R_{ij} = \frac{V_{cav}}{V} \frac{1}{k_0} (A_1 \delta_{ij} + A_2 n_i n_j),$$  \hspace{1cm} (4.2)

where the shape factors $A_1$ and $A_2$ are known (elementary) functions of the aspect ratio $\gamma$ (see Kachanov et al. (2001) and Sevostianov & Kachanov (2002) for details).

In the limit of a circular crack of radius $a(\gamma \to 0)$,

$$H^R = \frac{1}{k_0} \frac{8}{3} \frac{a^3}{V} n n.$$  \hspace{1cm} (4.3)

Similarly to the elasticity problem, the strongly oblate pores (aspect ratios up to $\gamma = 0.15$) can be replaced, with good accuracy, by cracks, as far as their impact on the overall conductivities is concerned.

In the approximation of (thermally) non-interacting cracks, each crack is subject to the same far-field temperature gradient unperturbed by the presence of other cracks. The effective conductivity tensor $K_{ij}$ is then expressed in terms of the same crack-density tensor $\alpha_{ij}$ that enters the elasticity problem (see (2.7)):

$$k_0/K_{ij} = \delta_{ij} + \frac{8}{3} \alpha_{ij}.$$  \hspace{1cm} (4.4)

In the case of the annular crack, the resistivity-contribution tensor can be related to that of the circular crack. In this paper, the conductivity problem for material containing an annular crack is solved numerically using the commercial finite-element code PDEase®. We fixed the outer radius $a$ and calculated the effective resistivity for various values of the inner radius $c$. Figure 6a illustrates the typical mesh generated by PDEase® (in this particular picture $\lambda = c/a = 0.6$). As the result, we received the relative effective resistivity change $k_0 H^R$ as a function of the ‘island parameter’ $\lambda$ (table 1). The radius of the effective circular crack was then calculated using (4.3). Figure 6b gives the radius $R_{\text{eff}}$ of the ‘equivalent’ circular crack that produces the same resistivity change as the annular crack.

We have to clarify why the conductivity problem (which is simpler than the elasticity problem) is solved numerically. In principle, the same approach, as described in §3, can be used to construct the solution. However, it requires the knowledge of the quantity analogous to the SIF in solid mechanics. To the best of our knowledge, the appropriate methodology has not yet been developed. We do not consider this problem in the present paper.

Figure 6. (a) Typical mesh generated by PDEase® for calculation of the effective resistivity (in this particular picture $\lambda = c/a = 0.6$); (b) radius of the equivalent circular crack for the conductivity problem.

5. Cross-property relation for material containing multiple annular cracks

Comparison of figures 4a and 6b leads to the important conclusion that differences in radii of the equivalent circular cracks, calculated for the elastic and for the conductive...
problems, do not exceed 3%. Therefore, annular cracks can be replaced by the same circular ones for both elastic and conductive problems. It allows us to conclude that, in the framework of the non-interaction approximation, the effective compliances of a material containing annular cracks can be explicitly expressed in terms of the effective conductivities (cross-property relations). Indeed, since equivalent circular cracks can be used both for elasticity and conductivity problems, excluding components $\alpha_{11}$ and $\alpha_{33}$ of the crack-density tensor from (4.4) and substituting them into (2.6) yields the following relation for effective compliances:

$$S = S_0 + \frac{2(1 - \nu_0^2)}{(2 - \nu_0)E_0} [(k_0K^{-1} - I) \cdot J + J \cdot (k_0K^{-1} - I)].$$  \hfill (5.1)

In particular, effective Young’s moduli $E_i$ are given in terms of corresponding conductivities $k_i$ by the following simple formula:

$$\frac{E_0 - E_i}{E_i} = \frac{4(1 - \nu_0^2) k_0 - k_i}{2 - \nu_0} \frac{k_i}{k_0}.$$  \hfill (5.2)

Note that these cross-property correlations do not require any knowledge of the porous-space geometry. The advantage of the explicit cross-property connections is that using the available data on one of the properties, which is easier to measure (say, electric conductivity), we can estimate another one that is more difficult to measure (say, anisotropic elastic constants).

6. Conclusions

This paper focuses on material containing annular cracks, defects which are bounded by fourth-order surfaces (rather than second-order surfaces, such as ellipsoids) and, therefore, cannot be described in terms of Eshelby tensors. The compliance contribution tensor for an annular crack is calculated on the basis of SIFs. The effective circular crack, a crack which yields the same change in material properties as the given annular crack, is calculated for a problem of elasticity as well as for one of thermal conductivity. It is shown that the same circular crack can be used in both of these problems.

This finding allows one to formulate an explicit cross-property relation for materials containing annular cracks. The cross-property relation is derived in the framework of a non-interaction approximation. However, experimental results of Sevostianov et al. (2002) and Bogarapu & Sevostianov (2002) show that the interactions affect both elastic and electric properties of a porous/microcracked material in a similar way, so that the cross-property correlations derived in the framework of the non-interaction approximation continue to hold for highly porous materials. Note that this idea was first suggested by Bristow (1960) for a material with randomly oriented cracks.

A typical example of a material containing annular cracks (plasma-sprayed coating) is discussed. It is shown that the existence of islands has a pronounced effect on the effective elastic (and conductive) properties of the coatings. In particular, the existence of islands explains the permanent substantial overestimation of the effective properties of plasma-sprayed coatings calculated under the assumption that all the cracks are circular.

The research is supported by General Electric Corporative Research and Development (Schenectady, NY, USA) and by Alstom AG (Baden, Switzerland). The author thanks the anonymous reviewers for a number of very helpful remarks.

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