DEPENDENCE OF THE EFFECTIVE THERMO-MECHANICAL PROPERTIES OF A PARTICULATE COMPOSITE ON PARTICLES SIZE

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1. Introduction. In various composites containing foreign particles, the latter are usually surrounded by thin interface layers. In most cases, their thickness is much smaller than the inclusion sizes and the overall elasticity and conductivity are not significantly affected by the presence of interfaces. However, if the typical size of reinforcement particles in a composite is of order of nanometers, the thickness of the inclusion/matrix interphase zone is usually comparable to the particle sizes and its effect on the effective properties of a composite may be substantial. We note that the interlayer has thickness of the order of 1-2 nm (Mütschele and Kirchheim (1987)), i.e. several interatomic spacing. The thickness is approximately constant and can be viewed as intrinsic characteristics of the pair of materials. Although this scale is at the limit of applicability of continuum mechanics, we assume that, as far as the effective, i.e. the volume average, properties are concerned, the continuum mechanics approach can still be used. Whereas the interface thickness is approximately constant from one particle to another, the sizes of the "core" nanoparticles vary. Therefore, the overall thermo-mechanical properties of the composite will depend on the distribution of the ratio of the layer thickness to the inclusion size. Analysis of this dependence is one of the goals of the present work. The problem arises of identifying those parameters of the interface (its relative thickness, property variability across the thickness) that produce a dominant effect on the overall elasticity or overall conductivity. We address it by first identifying an equivalent *homogeneous* inclusion that, being placed in the matrix would produce the same contribution to the overall properties and then considering the composite with equivalent homogeneous inclusions.

2. Equivalent homogeneous inclusion. We denote by C one of the elastic moduli, either the bulk one, K, or the shear one, G. The interface layer has the inner and the outer radii r_0 and $r_1 = r_0 + h$, respectively (Fig. 1). The inner core of radius r_0 has modulus C_* and the interface modulus varies across the thickness: $C^i = C^i(r)$. We aim at finding modulus $\overline{C} = \overline{C}(r_1)$ of the equivalent homogeneous inclusion of radius r_1.

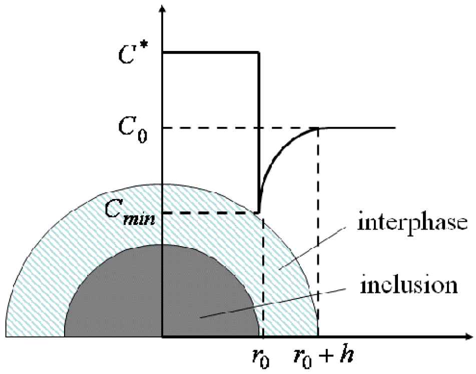

Figure 1. Structure of a spherical inhomogeneity of radius r_0 with functionally graded interphase zone of thickness *h*. Elastic modulus (either bulk or shear) or thermal conductivity of the inhomogeneity is C^*, corresponding property of the interphase zone varies from C_{min} to its value for the matrix material C_0.

We consider a certain "current" radius $r_0 < r < r_1$ and then add an incremental layer dr of the interface material, $r \to r + dr$, assuming that the inclusion of radius r is homogeneous (homogenized at the previous step). To find the corresponding increment of modulus of the equivalent homogeneous inclusion, we model this enlargement by placing the inclusion of radius r into a matrix that has the property of the interface $C^i(r)$. Volume fraction of the mentioned inclusion in the matrix is the ratio of the volume of the inclusion of radius r to the volume of the enlarged inclusion of radius $r + dr$. It is close to unity and, to the first order, is $1 - 3dr/r$.

Applying the technique of Shen and Li (2003) to the HS lower bound leads to the following differential equations for the moduli $\overline{K}$, $\overline{G}$ of the equivalent homogeneous inclusion:

$$\frac{d\overline{K}}{dr} = -\frac{3}{r}\frac{\left(\overline{K}(r) - K^i(r)\right)}{1+\alpha_K}\left(\alpha_K + \frac{\overline{K}(r)}{K^i(r)}\right)$$

$$\frac{d\overline{G}}{dr} = -\frac{3}{r}\left(\overline{G}(r) - G^i(r)\right)\left[1 + \alpha_G \frac{\overline{G}(r) - G^i(r)}{G^i(r)}\right]$$

with initial conditions $\bar{K}(r_0)=K^*$, $\bar{G}(r_0)=G^*$, where $\alpha_K=2\dfrac{1-2\nu_0}{1+\nu_0}$, $\alpha_G=\dfrac{2}{25}\dfrac{4-7\nu_0}{3-5\nu_0}$. In the solution, one should set $r=r_1=r_0+h$, where h is the interface thickness. Assuming the power law variation of the moduli across the inter interphase thickness

$$K(r)=K_0+(K_{min}-K_0)(r/r_0)^{-\beta};$$

$$G(r)=G_0+(G_{min}-G_0)(r/r_0)^{-\beta}$$

where the power exponent

$$\beta=\left|\frac{1}{ln(1+h/r)}ln\left(\frac{\delta C_0}{C_0-C_{min}}\right)\right| \quad (2.8)$$

is chosen in such a way that the properties are continuous at the inner boundary and are almost matched to the ones of the matrix (to within small parameter δ) at the outer boundary, the solution for the differential equations can be obtained in the form of hypergeometric functions (Sevostianov and Kachanov, 2007). It is plotted in Fig 2.

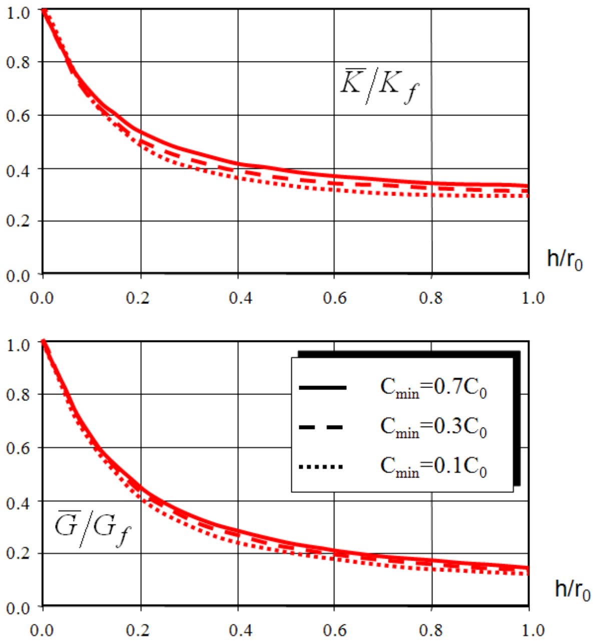

Figure 2. Effective normalized bulk and shear moduli of a spherical diamond inhomogeneity of radius r_0 embedded in copper matrix with functionally graded interphase zone of thickness *h*. Moduli are calculated at different values of C_{min}

For thermal expansion coefficient the differential equation has the form (Sevostianov, 2007)

$$\frac{d\bar{\alpha}}{dr}=-\frac{3}{r}\frac{\left(\bar{\alpha}(r)-\alpha^i(r)\right)}{1+\lambda}\left(\frac{K^i(r)}{\bar{K}(r)}\lambda+1\right)$$

where $\lambda=2(1-2\nu_0)/(1+\nu_0)$.

3. Effective properties of a composite reinforced with structured inhomogeneities. We consider now the effective TPC of a composite with "structured" inclusions and replace them by the equivalent homogeneous ones. We denote the matrix properties by subscript "0" and properties of the equivalent homogeneous inclusions – by an overbar. First, to estimate the effective bulk modulus, we use method of the effective field of Kanaun-Levin (see Kanaun and Levin, 2008 for a review) where a representative inhomogeneity is placed into a certain effective thermoelastic field. The main assumption of this method is that the effective field acting on each inhomogeneity is equal to the average over the entire composite (i.e. over matrix and inhomogeneities). In the framework of the effective field method, the effective bulk modulus of the composite can be calculated as

$$K_{eff}=K_0+\frac{c'(\bar{K}-K_0)(3K_0+4G_0)}{(3K_0+4G_0)+3(1-c')(\bar{K}-K_0)}\equiv K_0+c'A$$

$$G_{eff}=G_0+\frac{5c'G_0(\bar{G}-G_0)(3K_0+4G_0)}{5G_0(3K_0+4G_0)+6(1-c')(\bar{G}-G_0)(K_0+2G_0)}$$

$$\equiv G_0+c'B$$

where c' is the adjusted volume fraction of inhomogeneities, that includes interphase layers. The overall thermal expansion coefficient can then be obtained as

$$\alpha_{eff}=\alpha_0+\frac{c'(\bar{\alpha}-\alpha_0)\bar{K}(3K_0+4G_0)}{K_0\left[4G_0(1-c')+\bar{K}(3+2c')-2c'K_0\right]}$$

$$\equiv\alpha_0+c'D$$

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