Recent Progress in the Description of Inelastic Behaviour of Materials with Microdefects

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ABSTRACT

For solids containing microdefects such as cracks, inhomogeneities, voids, or gas bubbles, the overall effective moduli are estimated. Two possible extreme cases are discussed: (1) when defects are randomly distributed throughout an elastic matrix, and (2) when this distribution is periodic. It is shown that the assumption of periodic distribution leads to results which are in very good accord with experiments. These results are used to estimate overall moduli of type 316 stainless steel subjected to neutron irradiation.

1. Introduction

The presence of microcracks, inclusions, and other stress concentrators in rocks, concrete, and other materials reduces considerably their strength. Similarly, the formation and growth of voids and gas bubbles due to neutron irradiation affect the strength and ductility of metals. In the application to nuclear engineering, structural elements consisting of materials of this kind are often designed in such a manner that they undergo only small deformations. Hence, infinitesimal deformation theories may be used. Nevertheless, the presence and evolution of microdefects render the overall response nonlinear and history-dependent, even when a linearly elastic matrix which contains microdefects is involved.

To obtain useful results, one may consider two limiting models: (1) The microdefects are randomly distributed within the elastic matrix, and (2) the microdefects are periodically distributed within the matrix. The actual case, of course, will fall somewhere between these two limits. In this work, some recent results on both randomly and periodically distributed cracks and voids in a linearly elastic matrix are summarized. The results for periodically distributed voids are then used to estimate the overall bulk and shear moduli of irradiated stainless steel for various neutron fluences.

2. Randomly Distributed Defects

Defects which may be voids, cracks, or second-phase particles are often randomly distributed throughout the solid. When their density is small, their interaction, though important, may not be of the first order of significance in characterizing the overall response. For problems of this kind the self-consistent method, or a version of it, has been extensively used by many researchers; see, MacKenzie [1], Hershey [2], Kerner [3], Kröner [4,5], Budiansky [6], Hill [7,8], Watt et al. [9], Willis [10,11], and Mura [12] who reviews the literature and presents a detailed account. The basic assumption of this method is that a defect is affected by the presence of all other defects through the response of an effective homogeneous matrix which has the same instantaneous moduli as those of the overall composite. Hence, in order to calculate the stress and strain fields associated with one defect, this defect is placed within a homogeneous matrix of the overall instantaneous moduli, and a linearly elastic calculation is performed. This calculation is further simplified considerably by assuming that the defect has an ellipsoidal geometry. It has been shown by Eshelby [13] that, if an ellipsoidal region in an unbounded linearly elastic solid undergoes a transformation which in the absence of the surrounding matrix results in a uniform transformation strain, ϵ^*_{ij}, then in the presence of the constraint imposed by the surrounding elastic matrix, the strain in the ellipsoid is still uniform, but is given by $\epsilon_{ij} = S_{ijk\ell}\epsilon^*_{k\ell}$, where $S_{ijk\ell}$ is a constant tensor depending on the elastic moduli (the Poisson ratio only for the isotropic matrix) of the matrix and on the geometry of the ellipsoid; here and in the sequel a fixed rectangular Cartesian coordinate system is implied, coordinate axes are denoted by x_i, indices take on values 1, 2, 3, and repeated indices are summed.

In many applications the defects may not be ellipsoidal, or the ellipsoidal approximation to the actual geometry may not be an adequate description. Z-shaped cracks are such examples. For cavities, or for open or closed cracks, a different approach has been recently developed by Horii and Nemat-Nasser [14], which applies to any geometry. In this section this method is briefly reviewed.

Consider a solid of volume V and external surface S which supports tractions $\bar{\sigma}_{ij}n_j$, where n_j is the exterior unit normal, and

$$\bar{\sigma}_{ij} = \frac{1}{V} \int_V \sigma_{ij} \, dV \tag{2.1}$$

is the average stress. We confine, for the moment, our attention to inclusions and let f denote their volume fraction. Then,

$$\bar{\sigma}_{ij} = (1 - f)\bar{\sigma}^M_{ij} + f \, \bar{\sigma}^I_{ij} \, , \tag{2.2}$$

where superscripts M and I denote the averages taken over the matrix and the inclusions, respectively. If $\bar{\epsilon}_{ij}$ is the average strain, then

$$\bar{\epsilon}_{ij} = (1 - f)\bar{\epsilon}^M_{ij} + f \, \bar{\epsilon}^I_{ij} \, , \tag{2.3}$$

where again, M and I identify the averages over matrix and inclusions. Now it is easy to show that when the inclusions are stress-free <u>cavities</u> (or frictional cracks), we have

$$f \, \bar{\epsilon}^I_{ij} = \frac{1}{V} \int_{S^I} \frac{1}{2} (u_i n_j + u_j n_i) dS = H_{ijk\ell} \, \bar{\sigma}_{k\ell} \, , \tag{2.4}$$

where S^I is the surface of all inclusions, u_i is the displacement field, and $H_{ijk\ell}$ is a constant tensor (to be calculated). Furthermore, if $D_{ijk\ell}$ is the compliance tensor of the homogeneous matrix,

$$\bar{\epsilon}^M_{ij} = D_{ijk\ell} \, \bar{\sigma}^M_{ij} \, . \tag{2.5}$$

From (2.2) to (2.5) it readily follows that

$$D^*_{ijk\ell} = D_{ijk\ell} + H_{ijk\ell} \, , \tag{2.6}$$

where $D^*_{ijk\ell}$ is the overall compliance of the solid; in [14] this is denoted by $\bar{D}_{ijk\ell}$.

For cavities and cracks, $H_{ijk\ell}$ can be calculated directly from (2.4), and therefore, eq. (2.6) can be used to estimate the overall compliance. Observe that this result also applies when closed frictional cracks are involved. Examples of this kind are given by Horii and Nemat-Nasser [14].

For an ellipsoidal cavity, $H_{ijk\ell}$ coincides with Hill's [7] $V^I Q_{ijk\ell}{}^{-1}$, where V^I is the volume of the inclusion.

To apply the self-consistent method, a typical cavity or crack is first considered, and the corresponding tensor $H_{ijk\ell}$ is calculated from (2.4), assuming that the cavity is embedded in a homogeneous matrix of (yet unknown) overall moduli. Then the overall $H_{ijk\ell}$ is calculated by averaging the results of one cavity over all shapes and orientations of cavities and cracks. It is this final overall $H_{ijk\ell}$ which is used in eq. (2.6).

Consider as an example a solid that contains randomly distributed penny-shaped cracks. When all cracks are open, the overall response would be isotropic. Let a be the average crack radius, N be the number of cracks per unit volume, and define a crack density parameter f, by

$$f = a^3 N \, . \tag{2.7}$$

Then the overall Young modulus E^* and the Poisson ratio ν^* are obtained from (2.6) to be

$$\frac{E^*}{E} = 1 - f \, \frac{16(1 - \nu^{*2})(10 - 3\nu^*)}{45(2 - \nu^*)} \, , \tag{2.8}$$

$$f = \frac{45(\nu - \nu^*)(2 - \nu^*)}{16(1 - \nu^{*2})[10\nu - \nu^*(1 + 3\nu)]} , \qquad (2.9)$$

where E and ν are the Young modulus and the Poisson ratio of the matrix material. These equations were first obtained by Budiansky and O'Connell [15] using a different method.

As a second example, consider a plane strain problem of a rock sample which contains randomly distributed cracks. When the cracks are filled with liquid, one may assume the coefficient of friction to be zero. On the other hand, another limiting situation would be to assume a very large coefficient of friction, so that as soon as a crack is closed, it cannot slide. These two limiting cases will then bound the actual response, where some closed cracks may undergo frictional sliding. A typical example calculated by the self-consistent method is given in Fig. 1 for plane strain. (For further discussion, see Horii and Nemat-Nasser [14].) In this figure, μ is the coefficient of friction, τ (positive) is the shear stress, and p is the mean stress (positive when tensile, and negative when compressive). G^* is the average overall shear modulus, and G is that of the isotropic matrix. The Poisson ratio for the matrix is assumed to be 0.3. f is defined by (2.7).

3. Periodically Distributed Defects

In the preceding section the limiting case of total disorder, i.e. random distribution of defects, was briefly reviewed. The other extreme case is a complete order, i.e. a periodic distribution of defects.

When the density of voids, inclusions, or cracks is very high, the interaction among them becomes such a dominant factor in dictating the overall response, that the assumption of periodic distribution becomes quite reasonable. Indeed, except at very low volume fraction of inclusions and voids, the self-consistent method invariably underestimates the overall moduli for porous solids. On the other hand, calculations based on the assumption of periodic distributions produce results in amazingly good accord with experimental observations; see, Nemat-Nasser et al. [16].

Consider a solid that consists of parallelepiped unit cells of dimensions Λ_i, i=1,2,3. Let each cell contain a collection of voids or inclusions with total volume V^I. If, in the absence of any applied loads, variable transformation strains $\varepsilon^*_{ij}(\underset{\sim}{x})$ are prescribed in V^I in an otherwise homogeneous body, then one can exploit the periodicity of these transformation strains, and show that in the presence of the surrounding linearly elastic matrix, the strains are

$$\varepsilon_{jk}(\underset{\sim}{x}) = \frac{1}{V} \sum_{n_p=0}^{\pm\infty}{}' g_{jkmn}(\underset{\sim}{\xi}) \int_{V^I} \varepsilon^*_{mn}(\underset{\sim}{x}') \, e^{i\underset{\sim}{\xi}\cdot(\underset{\sim}{x}-\underset{\sim}{x}')} d\underset{\sim}{x}' , \qquad (3.1)$$

where a prime on $\sum$ indicates that $n = (n_p n_p)^{\frac{1}{2}} = 0$ is excluded in the summation. The fourth order tensor $g_{jkmn}(\underset{\sim}{\xi})$ is a homogeneous function of degree zero in $\xi_j = 2\pi n_j/\Lambda_j$ (no sum on j), depending only on the elasticity tensor, $\underset{\sim}{C}$, of the matrix. For isotropic case,

$$C_{ijk\ell} = \mu\,(\delta_{ik}\delta_{j\ell} + \delta_{i\ell}\delta_{jk}) + \lambda\delta_{ij}\delta_{k\ell} , \qquad (3.2)$$

we obtain

$$g_{ijk\ell}(\underset{\sim}{\xi}) = \frac{1}{2\xi^2}\left\{\xi_j(\delta_{i\ell}\xi_k + \delta_{ik}\xi_\ell) + \xi_i(\delta_{j\ell}\xi_k + \delta_{jk}\xi_\ell)\right\}$$

$$- \frac{1}{1-\nu}\,\frac{\xi_i\xi_j\xi_k\xi_\ell}{\xi^4} + \frac{\nu}{1-\nu}\,\frac{\xi_i\xi_j}{\xi^2}\,\delta_{k\ell}\,, \tag{3.3}$$

$$\xi^2 = \xi_k\xi_k\,, \tag{3.4}$$

where λ and μ are the Lamé constants and ν is the Poisson ratio of the matrix. Observe that the effect of the geometry can be separated from that of the material parameter, ν, if we introduce

$$g_{ijk\ell}(\underset{\sim}{\xi}) = g^{(1)}_{ijk\ell}(\underset{\sim}{\xi}) - \frac{1}{1-\nu}\, g^{(2)}_{ijk\ell}(\underset{\sim}{\xi}) + \frac{\nu}{1-\nu}\, g^{(3)}_{ijk\ell}(\underset{\sim}{\xi})\,, \tag{3.5}$$

where

$$g^{(1)}_{ijk\ell}(\underset{\sim}{\xi}) = \frac{1}{2}\left\{\bar{\xi}_j(\delta_{i\ell}\bar{\xi}_k + \delta_{ik}\bar{\xi}_\ell) + \bar{\xi}_i(\delta_{j\ell}\bar{\xi}_k + \delta_{jk}\bar{\xi}_\ell)\right\}\,, \tag{3.6}$$

$$g^{(2)}_{ijk\ell}(\underset{\sim}{\xi}) = \bar{\xi}_i\bar{\xi}_j\bar{\xi}_k\bar{\xi}_\ell\,, \quad g^{(3)}_{ijk\ell}(\underset{\sim}{\xi}) = \bar{\xi}_i\bar{\xi}_j\,\delta_{k\ell}\,, \tag{3.7}$$

and

$$\bar{\xi}_i = \frac{\xi_i}{\xi}\,. \tag{3.8}$$

Equation (3.1) replaces Eshelby's equation $\epsilon_{ij} = S_{ijk\ell}\epsilon^*_{k\ell}$. Indeed, if the dimensions of the unit cell are allowed to go to infinity, and the region V^I is ellipsoidal, one may show that eq. (3.1) reduces to Eshelby's result.

To apply (3.1), let the overall stress σ^0_{ij} be prescribed, and define the overall average strain by

$$\bar{\epsilon}_{ij} = D^*_{ijk\ell}\,\sigma^0_{k\ell}\,, \tag{3.9}$$

where $D^*_{ijk\ell}$ is yet unknown. Then, if the elasticity tensor of the inclusions is $C^I_{ijk\ell}$, one immediately obtains the following integral equations which define the transformation strains (see Nemat-Nasser et al. [16]):

$$\bar{\epsilon}_{ij} = A_{ijk\ell}\,\epsilon^*_{k\ell}(\underset{\sim}{x}) - \epsilon_{ij}(\underset{\sim}{x})\,, \tag{3.10}$$

where (3.1) is to be used, and

$$A_{ijk\ell} = \left(C_{ijmn} - C^I_{ijmn}\right)^{-1} C_{mnk\ell}\,. \tag{3.11}$$

For voids, $C^I_{ijk\ell}$ is zero, and $A_{ijk\ell}$ becomes the identity tensor.

The integral equations (3.10), (3.1), can be solved as accurately as desired; see, Nemat-Nasser et al. [16], Nemat-Nasser and Taya [17], and Iwakuma and Nemat-Nasser [18]. Indeed, an effective technique is to use a piece-wise constant approximation for the transformation strain, by dividing the region V^I into a finite number of subregions. The details of this and other solution techniques are extensively discussed and illustrated in [16,17,18].

When the overall strains are prescribed to be ϵ^0_{ij}, then the average overall stress is given by

$$\bar{\sigma}_{ij} = C^*_{ijk\ell}\,\epsilon^0_{k\ell}\,. \tag{3.12}$$

In this case, $\bar{\epsilon}_{ij}$ in the left-hand side of (3.10) must be replaced by ϵ^0_{ij}.

Note that $C^*_{ijk\ell}$ is the inverse of $D^*_{ijk\ell}$, as has been proved by Nemat-Nasser et al. [16].

To define these overall moduli, we equate the total elastic energy stored in a unit cell with $\frac{1}{2} VC^*_{ijk\ell}\epsilon^0_{ij}\epsilon^0_{k\ell}$, when the overall strains are prescribed, and with $\frac{1}{2} VD^*_{ijk\ell}\sigma^0_{ij}\sigma^0_{k\ell}$, when the overall stresses are prescribed. In this manner, one obtains

$$C^*_{ijk\ell}\ \epsilon^0_{k\ell} = C_{ijk\ell}\left[\epsilon^0_{k\ell} - f\ \bar{\epsilon}^*_{k\ell}\right] \tag{3.13}$$

when the overall strains are prescribed, and

$$D^*_{ijk\ell}\ \sigma^0_{k\ell} = D_{ijk\ell}\ \sigma^0_{k\ell} + f\ \bar{\epsilon}^*_{ij} \tag{3.14}$$

when the overall stress is prescribed. In these equations, f is the volume fraction of the inclusions and $\bar{\epsilon}^*_{ij}$ is the average transformation strain taken over V^I; ϵ^*_{ij} is zero outside V^I.

Observe that, in applying (3.13) or (3.14), only the average values of the transformation strains are needed. When the matrix is linearly elastic and isotropic, it can easily be shown that this average transformation strain tensor can be described in terms of several infinite series whose values depend only on the geometry of V^I, and which can be calculated once and for all, for given geometries. These infinite series can then be used in exactly the same way as Eshelby's tensor. For several common geometries, these infinite series have been calculated and tabulated by the author and coworkers [16,18]. It follows from these observations and from [16,18], that the average transformation strain is given by

$$\epsilon^0_{ij} = (A_{ijk\ell} - S_{ijk\ell})\ \bar{\epsilon}^*_{k\ell} \tag{3.15}$$

when strains are prescribed, where $S_{ijk\ell}$ involves several infinite series and depends on the geometry of V^I, and on the matrix moduli (the Poisson ratio for isotropic matrix). Combining (3.15) and (3.13), one arrives at

$$C^*_{ijk\ell} = C_{ijk\ell} - f\ C_{ijmn}\ (A_{mnk\ell} - S_{mnk\ell})^{-1} \tag{3.16}$$

which yields the overall moduli. Many examples are given in [16,18].

4. Overall Moduli of an Irradiated Solid

Voids are generated in solids that are exposed to neutron radiation; see, Bullough and Hayns [19] for a review and references. The elasticity of the solid therefore degrades as the void volume fraction increases. Recently, Afzali and Nemat-Nasser [20] estimated the moduli of such solids as functions of neutron fluence and temperature, using a semi-analytical semi-numerical approach. Further examination shows that the method overestimates considerably the effective moduli. Therefore, it is useful to reestimate these moduli, using the rather effective method that has been outlined in Section 3. To demonstrate that the assumption of periodicity is indeed very reasonable, we have reproduced in Figs.2(a),(b) calculations presented by Nemat-Nasser et al. [16] based on periodically distributed spherical voids, and compared results with some existing experimental data. As is seen, the calculation results are in excellent accord with those of experiment.

The relation between the void volume fraction, neutron fluence, and temperature is rather complicated, and here, as in [20], we use the empirical equations reported by Brager and Straalsund [21], i.e.

$$f = A(T)(\varphi t)^{B(T)} e^{C(T)}\ , \tag{4.1}$$

where f is in percent, φt is the neutron fluence in 10^{22} neutron/cm^2, and T is irradiation temperature in $^{\circ}$K. The empirical coefficients are (for type 316 stainless steel irradiated in EBR-II with neutron fluence in the range of $0.75 - 5.1 \times 10^{22}$ neutron/cm^2 at energies exceeding 0.1 MeV):

$$
\begin{aligned}
A(T) &= 0.48 + 9.2 \times 10^{-4}\,T \qquad \text{for } T \le 873\,, \\
&= 1.28 \qquad\qquad\qquad\quad\; \text{for } T \ge 873\,, \\
B(T) &= \frac{1.7}{1 + \exp[0.04(700 - T)]} + 0.72\,, \\
C(T) &= 28.09 - 0.02432\,T - 9440/T\,.
\end{aligned}
\tag{4.2}
$$

Assuming equally spaced spherical voids, we show in Fig. 3 our new estimates of the overall bulk and shear moduli as functions of neutron fluence, for irradiation temperatures of 400°C and 500°C. As is seen, a change of temperature from 400°C to 500°C causes a dramatic reduction in the overall moduli in the higher neutron fluence range. Note that at both temperatures, the estimates shown in Fig. 3 are lower than those previously given by Afzali and Nemat-Nasser [20]. The present estimates are believed to be more accurate.

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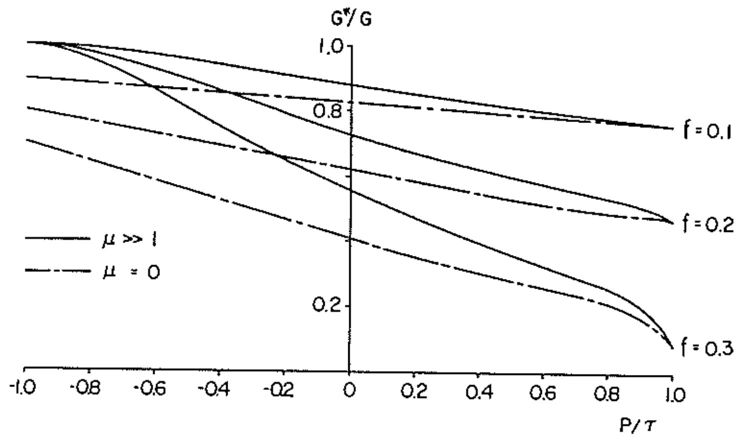

Fig. 1: Overall shear modulus vs. the stress ratio, p/τ, for indicated values of crack-density parameter $f = a^2N$; $\nu = 0.3$ (from Horii and Nemat-Nasser [14]).

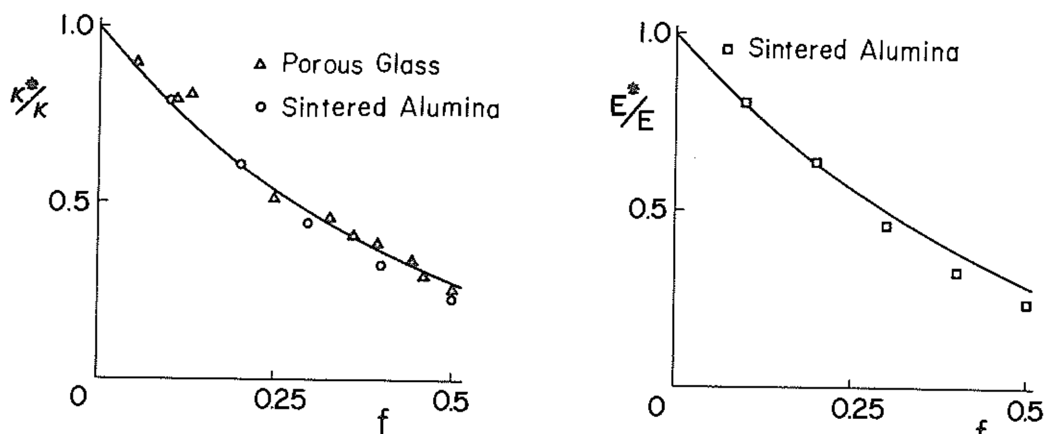

Fig. 2(a),(b): Comparison between experimental results and theoretical estimates of normalized bulk, κ^*/κ, and Young, E^*/E, moduli for a body with voids (from Nemat-Nasser et al. [16]).

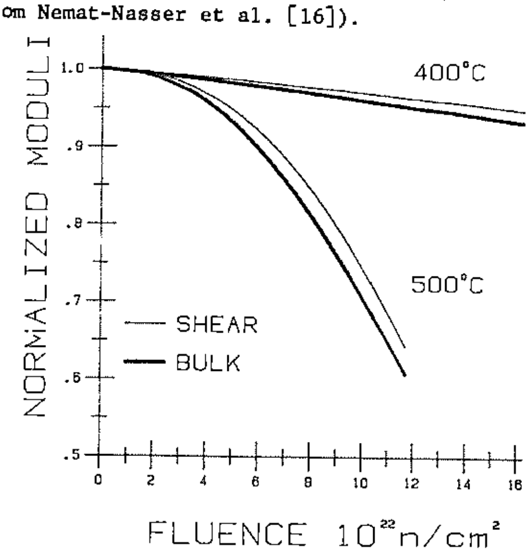

Fig. 3: Variation of normalized bulk, κ^*/κ, and shear, μ^*/μ, moduli with neutron fluence, φt, for indicated temperatures.