

ON THE RELATIONSHIP BETWEEN THE H-TENSOR AND THE CONCENTRATION TENSOR AND THEIR BOUNDS

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Abstract. For composite materials, two quantities that are useful for characterizing the contribution of inhomogeneities in a matrix material to the overall properties are (1) the *individual* H-tensor, \mathbf{H}_i , which describes the contribution of a single inhomogeneity and (2) the overall strain concentration tensor, which describes the relationship between the overall volumetric strain to the average strain of all of the inhomogeneities. In this paper, we develop a relationship expressing the *overall* H-tensor, \mathbf{H} , in terms of the overall strain concentration tensor. An important feature of the derivation is that it allows for rigorous upper and lower bounds on the overall H-tensor. In the special case that the inhomogeneities are all the same, with the same orientation, then $\mathbf{H} = \mathbf{H}_i$, and the results derived for \mathbf{H} also hold for \mathbf{H}_i .

Keywords: H-tensor, concentration-tensor, bounds

1 Introduction. A large number of materials consist of a base matrix material containing embedded particulates. Typically, one characterizes effective properties of heterogeneous materials by computing a constitutive relation between volume averaged field variables. The volume averaging takes place over a statistically representative sample of material, referred to in the literature as a representative volume element (RVE). The stiffness of a microheterogeneous material is characterized by a spatially variable elasticity tensor, \mathbf{IE} , while the effective stiffness tensor, \mathbf{IE}^* , is defined via

$$\langle \boldsymbol{\sigma} \rangle_{\Omega} = \mathbf{IE}^* : \langle \boldsymbol{\epsilon} \rangle_{\Omega}, \quad (1)$$

where

$$\langle \cdot \rangle_{\Omega} \stackrel{\text{def}}{=} \frac{1}{|\Omega|} \int_{\Omega} \cdot d\Omega, \quad (2)$$

and where $\boldsymbol{\sigma}$ and $\boldsymbol{\epsilon}$ are the stress and strain tensor fields within a RVE of volume $|\Omega|$.

The literature on this topic is immense, dating back to the early works of Maxwell [13], [14] and Lord Rayleigh [17]. For an extensive overview of random heterogeneous media, see Torquato [20] for more mathematical homogenization aspects, Jikov et al.[8] for more mathematical aspects, for solid-mechanics issues, Hashin [5], Markov [12], Mura [15], Nemat-Nasser and Hori [16], Huet [6], [7], for analyses of cracked media, Kachanov [9] and for computational aspects, Zohdi and Wriggers [21] and, recently, Ghosh [1], Ghosh and Dimiduk [2]. Two possible quantities for characterizing the contribution of the inhomogeneities in a matrix material are (1) H-tensors and

(2) strain concentration tensors, both of which describe the contribution of inhomogeneities in a matrix material to the overall properties. In this paper, we develop a relation expressing the H-tensor in terms of the strain concentration tensor, the overall effective property, the properties of the component materials and the volume fractions. This in turn allows for rigorous bounds on the overall H-tensor, and in some cases the individual H-tensor.

2 Overall H-tensor. The *individual* H-tensor, which was originally introduced to characterize the effective moduli of solids with cavities of various shapes by Kachanov et al [10], and extended by Kachanov and Sevostianov [11] to general inhomogeneities, allows for the identification of the strain in a second phase for a single second phase *i*th particle (inhomogeneity). In order to determine the individual H-tensor, one performs the following decomposition

$$\langle \boldsymbol{\epsilon} \rangle_{\Omega_{2i}} = \mathbf{IE}_1^{-1} : \langle \boldsymbol{\sigma} \rangle_{\Omega} + \langle \Delta \boldsymbol{\epsilon} \rangle_{\Omega_{2i}}, \quad (3)$$

where the individual H-tensor is defined via

$$\mathbf{H}_i : \langle \boldsymbol{\sigma} \rangle_{\Omega} = \langle \Delta \boldsymbol{\epsilon} \rangle_{\Omega_{2i}}, \quad (4)$$

and where $\langle \boldsymbol{\epsilon} \rangle_{\Omega_{2i}}$ is the average strain in the *i*th second phase (with domain Ω_{2i}), \mathbf{IE}_1^{-1} is the compliance of the first (matrix) phase, $\langle \boldsymbol{\sigma} \rangle_{\Omega}$ is the overall average stress, and $\langle \Delta \boldsymbol{\epsilon} \rangle_{\Omega_{2i}}$ characterizes the contribution of the *i*th second phase inhomogeneity to the average strain in the *i*th second phase. For an overview of the individual H-tensor, and its various properties, see Kachanov et al [10], Kachanov and Sevostianov [11] and Sevostianov et al [18]. In this work, we extend this definition to the entire group of second phase particles via

$$\langle \boldsymbol{\epsilon} \rangle_{\Omega_2} = \mathbf{IE}_1^{-1} : \langle \boldsymbol{\sigma} \rangle_{\Omega} + \langle \Delta \boldsymbol{\epsilon} \rangle_{\Omega_2}, \quad (5)$$

where $\langle \boldsymbol{\epsilon} \rangle_{\Omega_2}$ is the average strain in all of the second phase material (with domain Ω_2) and where we define overall H-tensor is defined via

$$\mathbf{H} : \langle \boldsymbol{\sigma} \rangle_{\Omega} = \langle \Delta \boldsymbol{\epsilon} \rangle_{\Omega_2}. \quad (6)$$

Remark: In the special case the inhomogeneities are all the same, with the same orientation, then the \mathbf{H}_i are all the same and

$$\mathbf{H} = \mathbf{H}_i, \quad (7)$$

which follows from

$$|\Omega_2| \mathbf{H} : \langle \boldsymbol{\sigma} \rangle_{\Omega} = |\Omega_2| \langle \Delta \boldsymbol{\epsilon} \rangle_{\Omega_2} = \sum_{i=1}^N |\Omega_{2i}| \langle \Delta \boldsymbol{\epsilon} \rangle_{\Omega_{2i}} = \sum_{i=1}^N |\Omega_{2i}| \mathbf{H}_i : \langle \boldsymbol{\sigma} \rangle_{\Omega}, \quad (8)$$

since $\sum_{i=1}^N |\Omega_{2i}| = |\Omega_2|$, where $|\Omega_{2i}|$ is the volume of the i th inhomogeneity (N in total), and $|\Omega_2|$ is the volume of all of the inhomogeneities. In this special case, all of the results for \mathcal{H} that will follow, also hold for \mathbf{H}_i .

3 Overall strain concentration tensor. Now consider the following identity for the overall strain

$$\langle \boldsymbol{\epsilon} \rangle_{\Omega} = \frac{1}{|\Omega|} \left(\int_{\Omega_1} \boldsymbol{\epsilon} d\Omega + \int_{\Omega_2} \boldsymbol{\epsilon} d\Omega \right) = v_1 \langle \boldsymbol{\epsilon} \rangle_{\Omega_1} + v_2 \langle \boldsymbol{\epsilon} \rangle_{\Omega_2}, \quad (9)$$

where Ω_1 can be considered as the domain of the matrix material and, as before, Ω_2 can be considered as the domain of all of the particulate material. Furthermore, for the overall stress

$$\langle \boldsymbol{\sigma} \rangle_{\Omega} = \frac{1}{|\Omega|} \left(\int_{\Omega_1} \boldsymbol{\sigma} d\Omega + \int_{\Omega_2} \boldsymbol{\sigma} d\Omega \right) = v_1 \langle \boldsymbol{\sigma} \rangle_{\Omega_1} + v_2 \langle \boldsymbol{\sigma} \rangle_{\Omega_2}. \quad (10)$$

Relatively straightforward algebra yields

$$\begin{aligned} \langle \boldsymbol{\sigma} \rangle_{\Omega} &= v_1 \langle \boldsymbol{\sigma} \rangle_{\Omega_1} + v_2 \langle \boldsymbol{\sigma} \rangle_{\Omega_2} \\ &= v_1 \mathbf{IE}_1 : \langle \boldsymbol{\epsilon} \rangle_{\Omega_1} + v_2 \mathbf{IE}_2 : \langle \boldsymbol{\epsilon} \rangle_{\Omega_2} \\ &= \mathbf{IE}_1 : (\langle \boldsymbol{\epsilon} \rangle_{\Omega} - v_2 \langle \boldsymbol{\epsilon} \rangle_{\Omega_2}) + v_2 \mathbf{IE}_2 : \langle \boldsymbol{\epsilon} \rangle_{\Omega_2} \\ &= (\mathbf{IE}_1 + v_2 (\mathbf{IE}_2 - \mathbf{IE}_1) : \mathbf{C}) : \langle \boldsymbol{\epsilon} \rangle_{\Omega} \end{aligned} \quad (11)$$

where

$$\underbrace{\left(\frac{1}{v_2} (\mathbf{IE}_2 - \mathbf{IE}_1)^{-1} : (\mathbf{IE}^* - \mathbf{IE}_1) \right)}_{\stackrel{\text{def}}{=} \mathbf{C}} : \langle \boldsymbol{\epsilon} \rangle_{\Omega} = \langle \boldsymbol{\epsilon} \rangle_{\Omega_2}. \quad (12)$$

We refer to \mathbf{C} as the overall strain concentration tensor.

4 Relating the overall H-tensor and strain concentration tensor. Taking Equation 5 and combining it with Equation 6, we have

$$\langle \boldsymbol{\epsilon} \rangle_{\Omega_2} = \mathbf{IE}_1^{-1} : \langle \boldsymbol{\sigma} \rangle_{\Omega} + \mathcal{H} : \langle \boldsymbol{\sigma} \rangle_{\Omega}, \quad (13)$$

and using the definition of the effective property

$$\langle \boldsymbol{\sigma} \rangle_{\Omega} = \mathbf{IE}^* : \langle \boldsymbol{\epsilon} \rangle_{\Omega} \quad (14)$$

yields

$$\langle \boldsymbol{\epsilon} \rangle_{\Omega_2} = \mathbf{IE}_1^{-1} : \langle \boldsymbol{\sigma} \rangle_{\Omega} + \mathcal{H} : (\mathbf{IE}^* : \langle \boldsymbol{\epsilon} \rangle_{\Omega}). \quad (15)$$

Combining Equation 15 with Equation 12

$$\mathbf{IE}_1^{-1} : \langle \boldsymbol{\sigma} \rangle_{\Omega} + \mathcal{H} : \mathbf{IE}^* : (\langle \boldsymbol{\epsilon} \rangle_{\Omega}) = \mathbf{C} : \langle \boldsymbol{\epsilon} \rangle_{\Omega}, \quad (16)$$

which can be solved to yield

$$\mathcal{H} = \left(\mathbf{C} : \mathbf{I}\mathbf{E}^{*-1} - \mathbf{I}\mathbf{E}_1^{-1} \right). \quad (17)$$

5 Special case of isotropy. In the case of isotropy we may write Equation 5 as

$$\langle \text{tr} \frac{\boldsymbol{\epsilon}}{3} \rangle_{\Omega_2} = \frac{1}{3\kappa_1} \langle \frac{\text{tr} \boldsymbol{\sigma}}{3} \rangle_{\Omega} + \langle \frac{\text{tr} \Delta \boldsymbol{\epsilon}}{3} \rangle_{\Omega_2}, \quad (18)$$

and

$$\langle \boldsymbol{\epsilon}' \rangle_{\Omega_2} = \frac{1}{2\mu_1} \langle \boldsymbol{\sigma}' \rangle_{\Omega} + \langle \Delta \boldsymbol{\epsilon}' \rangle_{\Omega_2}, \quad (19)$$

where $\boldsymbol{\epsilon} = \frac{\text{tr} \boldsymbol{\epsilon}}{3} \mathbf{1} + \boldsymbol{\epsilon}'$, $\boldsymbol{\sigma} = \frac{\text{tr} \boldsymbol{\sigma}}{3} \mathbf{1} + \boldsymbol{\sigma}'$, and $\boldsymbol{\sigma} = 3\kappa \frac{\text{tr} \boldsymbol{\epsilon}}{3} \mathbf{1} + 2\mu \boldsymbol{\epsilon}'$. Here we define

$$\mathcal{H}_{\kappa} \langle \frac{\text{tr} \boldsymbol{\sigma}}{3} \rangle_{\Omega} = \langle \frac{\text{tr} \Delta \boldsymbol{\epsilon}}{3} \rangle_{\Omega_2} \quad (20)$$

and

$$\mathcal{H}_{\mu} \langle \boldsymbol{\sigma}' \rangle_{\Omega} = \langle \Delta \boldsymbol{\epsilon}' \rangle_{\Omega_2}. \quad (21)$$

Furthermore, for the overall concentration tensor, we may write

$$C_{\kappa} \stackrel{\text{def}}{=} \frac{1}{v_2} \frac{\kappa^* - \kappa_1}{\kappa_2 - \kappa_1} \quad \text{and} \quad C_{\mu} \stackrel{\text{def}}{=} \frac{1}{v_2} \frac{\mu^* - \mu_1}{\mu_2 - \mu_1} \quad (22)$$

where $C_{\kappa} \langle \frac{\text{tr} \boldsymbol{\epsilon}}{3} \rangle_{\Omega} = \langle \frac{\text{tr} \boldsymbol{\epsilon}}{3} \rangle_{\Omega_2}$ and $C_{\mu} \langle \boldsymbol{\epsilon}' \rangle_{\Omega} = \langle \boldsymbol{\epsilon}' \rangle_{\Omega_2}$. In the case of isotropy, and using the definitions in Equations 20 and 21, we have

$$\mathcal{H}_{\kappa}(\kappa^*) \stackrel{\text{def}}{=} \frac{1}{3\kappa^*} \left(\frac{1}{v_2} \frac{\kappa^* - \kappa_1}{\kappa_2 - \kappa_1} - \frac{\kappa^*}{\kappa_1} \right) \quad (23)$$

and

$$\mathcal{H}_{\mu}(\mu^*) \stackrel{\text{def}}{=} \frac{1}{2\mu^*} \left(\frac{1}{v_2} \frac{\mu^* - \mu_1}{\mu_2 - \mu_1} - \frac{\mu^*}{\mu_1} \right). \quad (24)$$

6 Bounds on the overall H-tensor and concentration tensors. The two quantities $\mathcal{H}_{\kappa}(\kappa^*)$ and $\mathcal{H}_{\mu}(\mu^*)$ can be bounded by using effective property bounds of the form (assuming $\kappa_2 \geq \kappa_1$ and $\mu_2 \geq \mu_1$)

$$\kappa_1 \leq \kappa^{*, -} \leq \kappa^* \leq \kappa^{*, +} \leq \kappa_2 \quad (25)$$

and

$$\mu_1 \leq \mu^{*, -} \leq \mu^* \leq \mu^{*, +} \leq \mu_2. \quad (26)$$

Immediately inserting effective property bounds into Equations 23 and 24, we have for the H-tensor

$$\mathcal{H}_\kappa(\kappa^{*,-}) \leq \mathcal{H}_\kappa(\kappa^*) \leq \mathcal{H}_\kappa(\kappa^{*,+}) \quad (27)$$

and

$$\mathcal{H}_\mu(\mu^{*,-}) \leq \mathcal{H}_\mu(\mu^*) \leq \mathcal{H}_\mu(\mu^{*,+}). \quad (28)$$

Similarly, for the overall concentration tensors

$$C_\kappa(\kappa^{*,-}) \leq C_\kappa(\kappa^*) \leq C_\kappa(\kappa^{*,+}) \quad (29)$$

and

$$C_\mu(\mu^{*,-}) \leq C_\mu(\mu^*) \leq C_\mu(\mu^{*,+}). \quad (30)$$

For example, for tangible bounds, consider the widely used Hashin and Shtrikman bounds ([3],[4]), for isotropic materials with isotropic effective responses; for the bulk modulus,

$$\kappa^{*,-} \stackrel{\text{def}}{=} \kappa_1 + \frac{v_2}{\frac{1}{\kappa_2 - \kappa_1} + \frac{3(1-v_2)}{3\kappa_1 + 4\mu_1}} \leq \kappa^* \leq \kappa_2 + \frac{1 - v_2}{\frac{1}{\kappa_1 - \kappa_2} + \frac{3v_2}{3\kappa_2 + 4\mu_2}} \stackrel{\text{def}}{=} \kappa^{*,+}, \quad (31)$$

and for the shear modulus

$$\mu^{*,-} \stackrel{\text{def}}{=} \mu_1 + \frac{v_2}{\frac{1}{\mu_2 - \mu_1} + \frac{6(1-v_2)(\kappa_1 + 2\mu_1)}{5\mu_1(3\kappa_1 + 4\mu_1)}} \leq \mu^* \leq \mu_2 + \frac{(1 - v_2)}{\frac{1}{\mu_1 - \mu_2} + \frac{6v_2(\kappa_2 + 2\mu_2)}{5\mu_2(3\kappa_2 + 4\mu_2)}} \stackrel{\text{def}}{=} \mu^{*,+}, \quad (32)$$

where it is assumed that $\kappa_2 \geq \kappa_1$ and $\mu_2 \geq \mu_1$. Such bounds are considered the tightest known on isotropic effective responses, with isotropic two phase microstructures, when the only known data are the volume fractions and phase contrasts of the constituents.

7 “Dual” Quantities. One can also apply the preceding analysis the “dual” quantity, the so-called *individual* N-tensor, defined by Sevostianov and Kachanov [19],

$$\mathbf{N}_i : \langle \boldsymbol{\epsilon} \rangle_\Omega = \langle \Delta \boldsymbol{\sigma} \rangle_{\Omega_{2i}}, \quad (33)$$

where

$$\langle \boldsymbol{\sigma} \rangle_{\Omega_{2i}} = \mathbf{IE}_1 : \langle \boldsymbol{\epsilon} \rangle_\Omega + \langle \Delta \boldsymbol{\sigma} \rangle_{\Omega_{2i}}, \quad (34)$$

along with the *overall* N-tensor

$$\mathbf{N} : \langle \boldsymbol{\epsilon} \rangle_\Omega = \langle \Delta \boldsymbol{\sigma} \rangle_{\Omega_2}, \quad (35)$$

where

$$\langle \boldsymbol{\sigma} \rangle_{\Omega_2} = \mathbf{IE}_1 : \langle \boldsymbol{\epsilon} \rangle_\Omega + \langle \Delta \boldsymbol{\sigma} \rangle_{\Omega_2}. \quad (36)$$

By using the overall *stress* concentration tensors of the form $\bar{\mathbf{C}} : \langle \boldsymbol{\sigma} \rangle_{\Omega} = \langle \boldsymbol{\sigma} \rangle_{\Omega_2}$ (instead of overall strain concentration tensors, see Zohdi and Wriggers [21]), the analysis proceeds for the N-tensor as in the H-tensor case. Finally, we again highlight the special case remarked upon earlier in section 2 that, when the particles are all the same, with the same orientation, all of the results derived for \mathcal{H} also hold for \mathbf{H}_i and, in a similar manner, for \mathcal{N} and \mathbf{N}_i .

Acknowledgements: The author wishes to thank Prof. Mark Kachanov for his extremely helpful comments that substantially improved the paper.

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