



Joule-heating field phase-amplification in particulate-doped dielectrics

T.I. Zohdi

Department of Mechanical Engineering, University of California, Berkeley, CA 94720-1740, USA

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ABSTRACT

Doping dielectric materials with particulates for use in electronic device applications is wide-spread, particularly for energy-storage devices such as ultracapacitors and batteries. This work investigates the resulting distortion of the electrical fields in multiphase (particle and matrix) material systems. Of particular interest is to ascertain safe overall electrical loading conditions in order to avoid current overload in heterogeneous media. Specifically, it is important to determine the phase-wise Joule-type heating field, formed by the inner product of the current and electric fields. General estimates are developed, and two asymptotic cases are studied: (1) high-conductivity (“superconducting”) particles added to a lower relative-conductivity matrix and (2) low-conductivity (“insulator”) particles added to a higher relative-conductivity matrix. The expressions developed provide a relatively easy guide for the selection of dopants in dielectric material design.

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1. Introduction

Many electronic devices consist of an easily moldable matrix material which is doped with particulates with different dielectric constants, in order to tailor the overall dielectric response of the material for a specific application (Fig. 1). In the context of electrical materials, the microscale properties are characterized by a spatially variable electrical conductivity $\sigma(\mathbf{x})$. Typically, in order to characterize the structural-scale effective response of such materials, a relation between volume averages

$$\langle \mathbf{J} \rangle_{\Omega} = \sigma^* \cdot \langle \mathbf{E} \rangle_{\Omega}, \quad (1.1)$$

is formed, where $\langle \cdot \rangle_{\Omega} \stackrel{\text{def}}{=} c1|\Omega| \int_{\Omega} \cdot d\Omega$ is the volume averaging operator, \mathbf{J} is the current and \mathbf{E} is the electric field within a statistically representative volume element (RVE) of volume $|\Omega|$. The quantity, σ^* , is known as the effective conductivity, and is the property used in usual (homogenized) macroscale analyses.¹

Heterogeneous microstructures lead to a distortion of the electrical and current field within the material mixture. This leads to the fields becoming amplified within the material, which can lead to a variety of detrimental effects. An important quantity of interest is the amount of heat generated from an electrical field. The interconversions of various forms of energy (electromagnetic, thermal, etc) in a system are governed by the first law of thermodynamics,

$$\rho \dot{w} - \mathbf{T} : \nabla \dot{\mathbf{u}} + \nabla \cdot \mathbf{q} - H = 0, \quad (1.2)$$

where ρ is the mass density, w is the stored energy per unit mass, \mathbf{T} is Cauchy stress, \mathbf{u} is the displacement field, \mathbf{q} is heat flux, and H is the rate of electromagnetic energy absorbed due to Joule-heating (a source term)

$$H = a(\mathbf{J} \cdot \mathbf{E}), \quad (1.3)$$

E-mail address: zohdi@me.berkeley.edu

¹ One can also seek other effective quantities, such as the effective permittivity, $\langle \mathbf{D} \rangle_{\Omega} = \epsilon^* \cdot \langle \mathbf{E} \rangle_{\Omega}$, where \mathbf{D} is the electrical field flux.

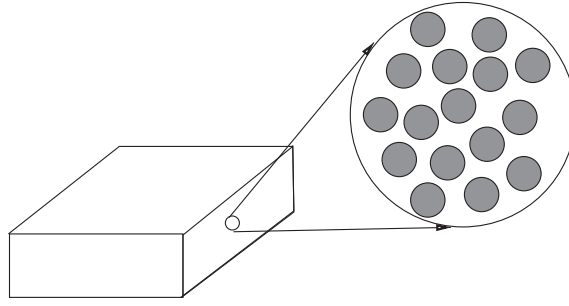


Fig. 1. A material with particulate additives.

where $0 \leq a \leq 1$ is an absorption constant. This standard form of Joule-heating is derived in the appendix. Thus, a material designer must seek ways by which to modify a base material in order to deliver a specified overall conductivity (for example by employing particulate additives), while simultaneously avoiding overheating.

Our objective in this paper is to determine the phase-wise levels of the Joule-field, denoted $H = \mathbf{J} \cdot \mathbf{E}$, in a heterogeneous three-dimensional continuum. The outline is as follows: (1) General expressions are developed for the Joule-heating field, $H = \mathbf{J} \cdot \mathbf{E}$ in a two-phase material, (2) The expressions are then specialized to isotropic cases, (3) Two asymptotic cases are then studied: (a) high-conductivity (“superconducting”) particles added to a lower relative-conductivity matrix and (b) low-conductivity (“insulator”) particles added to a higher relative-conductivity matrix, (4) Generalizations are developed for multiphase materials, such as coated particles embedded in a binding matrix and, (5) A summary is provided with extensions discussing numerical methods.

Remark. Another detrimental effect of large electrical fields is dielectric breakdown where, if the field is strong enough to mobilize free electrons that are present in a medium, they attain sufficiently large energies to dislodge other electrons, resulting in a large number of free electrons and positively charged ions. The dislodged electrons then repeat the procedure in a chain-like reaction manner. This effect can lead to electronic device failure.

2. Field decompositions for phase-wise load-levels

We consider a two-phase medium. One can determine the electric field “load level” carried by each phase by considering the following identities:

$$\langle \mathbf{E} \rangle_{\Omega} = \frac{1}{|\Omega|} \left(\int_{\Omega_1} \mathbf{E} d\Omega + \int_{\Omega_2} \mathbf{E} d\Omega \right) = v_1 \langle \mathbf{E} \rangle_{\Omega_1} + v_2 \langle \mathbf{E} \rangle_{\Omega_2} \tag{2.1}$$

and

$$\langle \mathbf{J} \rangle_{\Omega} = \frac{1}{|\Omega|} \left(\int_{\Omega_1} \mathbf{J} d\Omega + \int_{\Omega_2} \mathbf{J} d\Omega \right) = v_1 \langle \mathbf{J} \rangle_{\Omega_1} + v_2 \langle \mathbf{J} \rangle_{\Omega_2}, \tag{2.2}$$

where v_1 and v_2 are the volume fractions of phases 1 and 2 respectively, so that $v_1 + v_2 = 1$. Performing straightforward algebraic manipulations yields

$$\begin{aligned} \langle \mathbf{J} \rangle_{\Omega} &= v_1 \langle \mathbf{J} \rangle_{\Omega_1} + v_2 \langle \mathbf{J} \rangle_{\Omega_2} = v_1 \boldsymbol{\sigma}_1 \cdot \langle \mathbf{E} \rangle_{\Omega_1} + v_2 \boldsymbol{\sigma}_2 \cdot \langle \mathbf{E} \rangle_{\Omega_2} = \boldsymbol{\sigma}_1 \cdot (\langle \mathbf{E} \rangle_{\Omega} - v_2 \langle \mathbf{E} \rangle_{\Omega_2}) + v_2 \boldsymbol{\sigma}_2 \cdot \langle \mathbf{E} \rangle_{\Omega_2} \\ &= \underbrace{(\boldsymbol{\sigma}_1 + v_2(\boldsymbol{\sigma}_2 - \boldsymbol{\sigma}_1) \cdot \mathbf{C}_{E,2})}_{\boldsymbol{\sigma}^*} \cdot \langle \mathbf{E} \rangle_{\Omega}, \end{aligned} \tag{2.3}$$

where

$$\underbrace{\left(\frac{1}{v_2} (\boldsymbol{\sigma}_2 - \boldsymbol{\sigma}_1)^{-1} \cdot (\boldsymbol{\sigma}^* - \boldsymbol{\sigma}_1) \right)}_{\text{def } \mathbf{C}_{E,2}} \cdot \langle \mathbf{E} \rangle_{\Omega} = \langle \mathbf{E} \rangle_{\Omega_2}. \tag{2.4}$$

$\mathbf{C}_{E,2}$ is known as the electric field concentration tensor. Once either $\mathbf{C}_{E,2}$ or $\boldsymbol{\sigma}^*$ is known, the other can be determined. We have from Eq. (2.1)

$$\langle \mathbf{E} \rangle_{\Omega_1} = \frac{\langle \mathbf{E} \rangle_{\Omega} - v_2 \langle \mathbf{E} \rangle_{\Omega_2}}{v_1} = \frac{(\mathbf{1} - v_2 \mathbf{C}_{E,2}) \cdot \langle \mathbf{E} \rangle_{\Omega}}{v_1} \stackrel{\text{def}}{=} \mathbf{C}_{E,1} \cdot \langle \mathbf{E} \rangle_{\Omega}, \tag{2.5}$$

where

$$\mathbf{C}_{E,1} = \frac{1}{v_1}(\mathbf{1} - v_2\mathbf{C}_{E,2}) = \frac{\mathbf{1} - v_2\mathbf{C}_{E,2}}{1 - v_2}. \tag{2.6}$$

The concentration tensors indicate the amplification or reduction of the field within the phases relative to the overall field average.

For the overall current, we have

$$\langle \mathbf{J} \rangle_{\Omega} = \boldsymbol{\sigma}^* \cdot \langle \mathbf{E} \rangle_{\Omega} \Rightarrow \boldsymbol{\sigma}^{*-1} \cdot \langle \mathbf{J} \rangle_{\Omega} = \mathbf{C}_{E,2}^{-1} \cdot \langle \mathbf{E} \rangle_{\Omega_2} = \mathbf{C}_{E,2}^{-1} \cdot \boldsymbol{\sigma}_2^{-1} \cdot \langle \mathbf{J} \rangle_{\Omega_2}. \tag{2.7}$$

Thus,

$$\underbrace{\boldsymbol{\sigma}_2 \cdot \mathbf{C}_{E,2} \cdot \boldsymbol{\sigma}^{*-1}}_{\mathbf{C}_{J,2}} \cdot \langle \mathbf{J} \rangle_{\Omega} = \langle \mathbf{J} \rangle_{\Omega_2} \tag{2.8}$$

and

$$\mathbf{C}_{J,1} \cdot \langle \mathbf{J} \rangle_{\Omega} = \langle \mathbf{J} \rangle_{\Omega_1}, \tag{2.9}$$

where

$$\mathbf{C}_{J,1} = \frac{\mathbf{1} - v_2\mathbf{C}_{J,2}}{1 - v_2} = \boldsymbol{\sigma}_1 \cdot \mathbf{C}_{E,1} \cdot \boldsymbol{\sigma}^{*-1}. \tag{2.10}$$

In summary, we have the following concentration tensors:

- $\mathbf{C}_{E,2} \cdot \langle \mathbf{E} \rangle_{\Omega} = \langle \mathbf{E} \rangle_{\Omega_2}$ where $\mathbf{C}_{E,2} = \frac{1}{v_2}(\boldsymbol{\sigma}_2 - \boldsymbol{\sigma}_1)^{-1} \cdot (\boldsymbol{\sigma}^* - \boldsymbol{\sigma}_1)$,
- $\mathbf{C}_{E,1} \cdot \langle \mathbf{E} \rangle_{\Omega} = \langle \mathbf{E} \rangle_{\Omega_1}$ where $\mathbf{C}_{E,1} = \frac{1}{v_1}(\mathbf{1} - v_2\mathbf{C}_{E,2}) = \frac{\mathbf{1} - v_2\mathbf{C}_{E,2}}{1 - v_2}$,
- $\mathbf{C}_{J,2} \cdot \langle \mathbf{J} \rangle_{\Omega} = \langle \mathbf{J} \rangle_{\Omega_2}$ where $\mathbf{C}_{J,2} = \boldsymbol{\sigma}_2 \cdot \mathbf{C}_{E,2} \cdot \boldsymbol{\sigma}^{*-1}$,
- $\mathbf{C}_{J,1} \cdot \langle \mathbf{J} \rangle_{\Omega} = \langle \mathbf{J} \rangle_{\Omega_1}$ where $\mathbf{C}_{J,1} = \frac{\mathbf{1} - v_2\mathbf{C}_{J,2}}{1 - v_2} = \boldsymbol{\sigma}_1 \cdot \mathbf{C}_{E,1} \cdot \boldsymbol{\sigma}^{*-1}$.

Remark 1. Directly from Eqs. (2.1) and (2.2) one may write

$$\underbrace{v_1\mathbf{C}_{E,1}}_{\text{phase-1 contribution}} + \underbrace{v_2\mathbf{C}_{E,2}}_{\text{phase-2 contribution}} = \mathbf{1}, \tag{2.11}$$

$$\underbrace{v_1\mathbf{C}_{J,1}}_{\text{phase-1 contribution}} + \underbrace{v_2\mathbf{C}_{J,2}}_{\text{phase-2 contribution}} = \mathbf{1}.$$

The concentration tensors indicate the amplification of the field within the particle relative to the average of the field. There has been no approximation yet. The “effort” in the computations has shifted to the determination of the \mathbf{C} ’s. Classical methods approximate them. For example, the simplest approximation is $\mathbf{C}_{E,2} = \mathbf{1}$, which is the Wiener [17] upper bound ² (a constant E -field throughout the microstructure, while the Wiener lower bound yields $\mathbf{C}_{J,2} = \mathbf{1}$ (a constant J -field throughout the microstructure).

Remark 2. If the overall property is isotropic, as well as each of the constituents (for example a microstructure comprised of an isotropic binder embedded with randomly distributed isotropic particles), then we have the following, $\mathbf{C}_{E,i} = C_{E,i}\mathbf{1}$, where, explicitly for a two-phase material

$$C_{E,1} = \frac{1}{1 - v_2} \frac{\sigma_2 - \sigma^*}{\sigma_2 - \sigma_1}, \tag{2.12}$$

and

$$C_{E,2} = \frac{1}{v_2} \frac{\sigma^* - \sigma_1}{\sigma_2 - \sigma_1}, \tag{2.13}$$

and $\mathbf{C}_{J,i} = C_{J,i}\mathbf{1}$, leading to

$$C_{J,1} = \frac{\sigma_1}{\sigma^*(1 - v_2)} \left(\frac{\sigma_2 - \sigma^*}{\sigma_2 - \sigma_1} \right), \tag{2.14}$$

$$C_{J,2} = \frac{\sigma_2}{\sigma^* v_2} \left(\frac{\sigma^* - \sigma_1}{\sigma_2 - \sigma_1} \right). \tag{2.15}$$

² The Wiener Bounds [17] for N -phases are $(\sum_{i=1}^N v_i \sigma_i^{-1})^{-1} \leq \sigma^* \leq \sum_{i=1}^N v_i \sigma_i$. Tighter estimates, including generalized N -phase Hashin–Shtrikman bounds, can be found, for example, in Torquato [16].

Remark 3. Recall, that the overall volume average of the electric field $\langle \mathbf{E} \rangle_\Omega$ in a RVE sample is equivalent to the loading on the boundary, for uniform loading conditions (see appendix).

3. The Joule-fields

3.1. Ergodic assumptions for the Joule-field

We shall utilize the following energy/power criterion

$$\langle H \rangle_\Omega = \langle \mathbf{J} \cdot \mathbf{E} \rangle_\Omega = \langle \mathbf{J} \rangle_\Omega \cdot \langle \mathbf{E} \rangle_\Omega, \quad (3.1)$$

which is referred to as an ergodicity condition in statistical mechanics (Kröner [8], Torquato [16]) and as a Hill-type condition in the solid mechanics literature (Hill [5]). This is essentially a statement that the micro-energy(power) must equal the macro-energy(power). Eq. (3.1) is developed by first splitting the current and electric fields into a purely fluctuating (zero mean) $\mathbf{J} = \langle \mathbf{J} \rangle_\Omega + \tilde{\mathbf{J}}$, where $\langle \tilde{\mathbf{J}} \rangle_\Omega = \mathbf{0}$ and $\mathbf{E} = \langle \mathbf{E} \rangle_\Omega + \tilde{\mathbf{E}}$ where $\langle \tilde{\mathbf{E}} \rangle_\Omega = \mathbf{0}$. By direct expansion of the system energy/power:

$$\langle (\langle \mathbf{J} \rangle_\Omega + \tilde{\mathbf{J}}) \cdot (\langle \mathbf{E} \rangle_\Omega + \tilde{\mathbf{E}}) \rangle_\Omega = \langle \mathbf{J} \rangle_\Omega \cdot \langle \mathbf{E} \rangle_\Omega + \langle \tilde{\mathbf{J}} \cdot \tilde{\mathbf{E}} \rangle_\Omega \quad (3.2)$$

since $\langle \tilde{\mathbf{J}} \rangle_\Omega = \mathbf{0}$ and $\langle \tilde{\mathbf{E}} \rangle_\Omega = \mathbf{0}$. The ergodicity assumption is that $\langle \tilde{\mathbf{J}} \cdot \tilde{\mathbf{E}} \rangle_\Omega \rightarrow 0$, as the volume, $|\Omega| \rightarrow \infty$ (relative to the inherent length-scales in the microstructure). The implication is that, as the sample becomes infinitely large, $\tilde{\mathbf{J}} \cdot \tilde{\mathbf{E}}$ is purely fluctuating and hence $\langle \tilde{\mathbf{J}} \cdot \tilde{\mathbf{E}} \rangle_\Omega = 0$. In other words, the product of two purely fluctuating random fields is also purely fluctuating.

Remark. Usually, a numerical analyst will apply uniform loading on a large sample, with the understanding that this idealization reproduces what a representative volume element (which is much smaller than the structural component of intended use) would experience within a structure. Uniform loading is an idealization and will be present within a vanishingly small microstructure relative to a finite-sized engineering (macro)structure. The macro/micro criterion is commonly used to help determine the appropriate heterogeneous material sample size for numerical effective property calculations (Zohdi [18,19] and Zohdi and Wriggers [20]).

3.2. Decomposition of the Joule-field

The Joule-fields can be written as

$$\langle H \rangle_{\Omega_i} \stackrel{\text{def}}{=} \langle \mathbf{J} \rangle_{\Omega_i} \cdot \langle \mathbf{E} \rangle_{\Omega_i} = \boldsymbol{\sigma}_i^{-1} \cdot \langle \mathbf{J} \rangle_{\Omega_i} \cdot \langle \mathbf{J} \rangle_{\Omega_i} = \boldsymbol{\sigma}_i \cdot \langle \mathbf{E} \rangle_{\Omega_i} \cdot \langle \mathbf{E} \rangle_{\Omega_i}, \quad (3.3)$$

or explicitly in terms of the overall fields

$$\langle H \rangle_{\Omega_i} \stackrel{\text{def}}{=} \langle \mathbf{J} \rangle_{\Omega_i} \cdot \langle \mathbf{E} \rangle_{\Omega_i} = (\mathbf{C}_{J,i} \cdot \langle \mathbf{J} \rangle_\Omega) \cdot (\mathbf{C}_{E,i} \cdot \langle \mathbf{E} \rangle_\Omega), \quad (3.4)$$

or purely the overall current field

$$\langle H \rangle_{\Omega_i} \stackrel{\text{def}}{=} \langle \mathbf{J} \rangle_{\Omega_i} \cdot \langle \mathbf{E} \rangle_{\Omega_i} = \boldsymbol{\sigma}_i^{-1} \cdot \langle \mathbf{J} \rangle_{\Omega_i} \cdot \langle \mathbf{J} \rangle_{\Omega_i} = \boldsymbol{\sigma}_i^{-1} \cdot (\mathbf{C}_{J,i} \cdot \langle \mathbf{J} \rangle_\Omega) \cdot (\mathbf{C}_{J,i} \cdot \langle \mathbf{J} \rangle_\Omega), \quad (3.5)$$

or purely the overall electric field

$$\langle H \rangle_{\Omega_i} \stackrel{\text{def}}{=} \langle \mathbf{J} \rangle_{\Omega_i} \cdot \langle \mathbf{E} \rangle_{\Omega_i} = \boldsymbol{\sigma}_i \cdot \langle \mathbf{E} \rangle_{\Omega_i} \cdot \langle \mathbf{E} \rangle_{\Omega_i} = \boldsymbol{\sigma}_i \cdot (\mathbf{C}_{E,i} \cdot \langle \mathbf{E} \rangle_\Omega) \cdot (\mathbf{C}_{E,i} \cdot \langle \mathbf{E} \rangle_\Omega). \quad (3.6)$$

4. Limits on fields

One can adopt various criteria for limits on the phase-wise field, for example:

- **Criterion # 1:** Limits on the electrical fields: $\|\langle \mathbf{E} \rangle_{\Omega_i}\| = \|\mathbf{C}_{E,i} \cdot \langle \mathbf{E} \rangle_\Omega\| \leq E_{i,crit}$, thus

$$\|\langle \mathbf{E} \rangle_{\Omega_i}\| \leq \|\mathbf{C}_{E,i}\| \|\langle \mathbf{E} \rangle_\Omega\| \leq E_{i,crit} \Rightarrow \|\langle \mathbf{E} \rangle_\Omega\| \leq \frac{E_{i,crit}}{\|\mathbf{C}_{E,i}\|}, \quad (4.1)$$

and in the case of isotropy ($\mathbf{C}_{E,i} = C_{E,i} \mathbf{1}$)

$$\|\langle \mathbf{E} \rangle_\Omega\| \leq \frac{E_{i,crit}}{C_{E,i}}, \quad (4.2)$$

- **Criterion # 2:** Limits on the current fields: $\|\langle \mathbf{J} \rangle_{\Omega_i}\| = \|\mathbf{C}_{J,i} \cdot \langle \mathbf{J} \rangle_\Omega\| \leq J_{i,crit}$, thus

$$\|\langle \mathbf{J} \rangle_{\Omega_i}\| \leq \|\mathbf{C}_{J,i}\| \|\langle \mathbf{J} \rangle_\Omega\| \leq J_{i,crit} \Rightarrow \|\langle \mathbf{J} \rangle_\Omega\| \leq \frac{J_{i,crit}}{\|\mathbf{C}_{J,i}\|}, \quad (4.3)$$

and in the case of isotropy ($\mathbf{C}_{J,i} = C_{J,i}\mathbf{1}$)

$$\|\langle \mathbf{J} \rangle_{\Omega}\| \leq \frac{J_{i,crit}}{C_{J,i}}, \quad (4.4)$$

• **Criterion # 3:** Limits on the Joule-fields: $\langle H \rangle_{\Omega_i} = \langle \mathbf{J} \rangle_{\Omega_i} \cdot \langle \mathbf{E} \rangle_{\Omega_i} = (\mathbf{C}_{J,i} \cdot \langle \mathbf{J} \rangle_{\Omega}) \cdot (\mathbf{C}_{E,i} \cdot \langle \mathbf{E} \rangle_{\Omega}) \leq J_{i,crit} E_{i,crit}$, thus $(\langle H \rangle_{\Omega} \stackrel{\text{def}}{=} \langle \mathbf{J} \rangle_{\Omega} \cdot \langle \mathbf{E} \rangle_{\Omega})$,

$$\langle H \rangle_{\Omega_i} = \langle \mathbf{J} \rangle_{\Omega_i} \cdot \langle \mathbf{E} \rangle_{\Omega_i} \leq \|\mathbf{C}_{E,i}\| \|\mathbf{C}_{J,i}\| \langle H \rangle_{\Omega} \Rightarrow \langle H \rangle_{\Omega} \leq \frac{J_{i,crit} E_{i,crit}}{\|\mathbf{C}_{E,i}\| \|\mathbf{C}_{J,i}\|}, \quad (4.5)$$

which in the case of isotropy becomes

$$\langle H \rangle_{\Omega} \leq \frac{J_{i,crit} E_{i,crit}}{C_{E,i} C_{J,i}}, \quad (4.6)$$

or, alternatively, in terms of currents (assuming $J_{i,crit} = \|\boldsymbol{\sigma}_i\| E_{i,crit}$), which collapses Eq. (4.3)

$$\langle H \rangle_{\Omega_i} = \boldsymbol{\sigma}_i^{-1} \cdot \langle \mathbf{J} \rangle_{\Omega_i} \cdot \langle \mathbf{J} \rangle_{\Omega_i} \leq \|\boldsymbol{\sigma}_i^{-1}\| \|\mathbf{C}_{J,i}\| \|\mathbf{C}_{J,i}\| \|\langle \mathbf{J} \rangle_{\Omega}\|^2 \Rightarrow \|\langle \mathbf{J} \rangle_{\Omega}\| \leq \frac{J_{i,crit}}{\|\mathbf{C}_{J,i}\|}, \quad (4.7)$$

which in the case of isotropy, this collapses to Eq. (4.4), or, alternatively, in terms of electrical fields (which collapses to Eq. (4.1))

$$\langle H \rangle_{\Omega_i} = \boldsymbol{\sigma}_i \cdot \langle \mathbf{E} \rangle_{\Omega_i} \cdot \langle \mathbf{E} \rangle_{\Omega_i} \leq \|\boldsymbol{\sigma}\| \|\mathbf{C}_{E,i}\| \|\mathbf{C}_{E,i}\| \|\langle \mathbf{E} \rangle_{\Omega}\|^2 \Rightarrow \|\langle \mathbf{E} \rangle_{\Omega}\| \leq \frac{E_{i,crit}}{\|\mathbf{C}_{E,i}\|}, \quad (4.8)$$

which in the case of isotropy, this collapses to Eq. (4.2).

We remark that Criterion #3 results from the product of Criterion #1 and Criterion #2. For either of the three criteria, because the concentration functions depend on $\boldsymbol{\sigma}^*$ and $\boldsymbol{\sigma}^* = \mathcal{F}(\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_2, \nu_2, \text{microstructure})$, we need to employ estimates for $\boldsymbol{\sigma}^*$, for example, using effective property bounding principles.

5. Utilization of effective property bounds

There are a number of methods to estimate the overall macroscopic properties of materials consisting of a matrix, containing a uniform distribution of particles, in terms of the individual phase volume fractions and properties. For an in depth review of such techniques and the general theory of random heterogeneous media, see Torquato [16] for general interdisciplinary discussions, Jikov et al. [6] for more mathematical aspects, Hashin [4], Mura [9], Nemat-Nasser and Hori [10] for solid mechanics inclined accounts of the subject, Sevostianov and Kachanov [15] for analyses of cracked media and Zohdi and Wriggers [20] for computational aspects.

A widely-used set of estimates (in fact, bounds) for isotropic materials (such as an isotropic matrix with randomly dispersed isotropic particles) are the Hashin–Shtrikman bounds (Hashin and Shtrikman [3])

$$\underbrace{\sigma_1 + \frac{\nu_2}{\frac{1}{\sigma_2 - \sigma_1} + \frac{1 - \nu_2}{3\sigma_1}}}_{\sigma^{*-}} \leq \sigma^* \leq \underbrace{\sigma_2 + \frac{1 - \nu_2}{\frac{1}{\sigma_1 - \sigma_2} + \frac{\nu_2}{3\sigma_2}}}_{\sigma^{*+}}, \quad (5.1)$$

where $\sigma_2 \geq \sigma_1$, ν_2 is the volume fraction of phase with the higher σ value (“phase 2” (σ_2) in the former expression) for the conductivity-mismatch. Such bounds are the tightest for isotropic effective responses, with isotropic two phase microstructures, where only the volume fractions and phase contrasts of the constituents are known. The lower bound is typically more accurate for microstructures where high-conductivity particles are surrounded by a low-conductivity matrix, while the upper bound is more accurate for a high-conductivity matrix surrounding low-conductivity particles. This can be explained qualitatively in the following manner. Consider a heterogeneous material with 50% low-conductivity material and 50% high-conductivity material. Now consider a case (Case 1) where the matrix material is made of the low-conductivity material and the particles are comprised of the high-conductivity material and the opposite case (Case 2) where the matrix material is made of the high conductivity material and the particles are comprised of the low conductivity material. The bounds in both cases are the same, however, the actual overall conductivity in Case 2 is clearly higher than the overall conductivity in Case 1. Clearly, Case 1 is more closely approximated by the upper bound and Case 1 is closer to the lower bound. In summary, since the true effective property lies between the upper and lower bounds, one can construct the following approximation:

$$\sigma^* \approx \phi \sigma^{*+} + (1 - \phi) \sigma^{*-}, \quad (5.2)$$

where $0 \leq \phi \leq 1$. ϕ is an unknown function of the microstructure. However, the general trends are that, for cases where the upper bound is more accurate, $\phi > \frac{1}{2}$, while for cases when the lower bound is more accurate, $\phi < \frac{1}{2}$. We now investigate these cases further.

Remark. There is a direct analogy to a the elastic properties of a material comprised of a stiff (high-conductivity) matrix with embedded soft (low conductivity) inclusions versus a material comprised of a soft (low conductivity) matrix containing hard (high-conductivity) inclusions.

6. Asymptotic limits: superconductors and insulators

6.1. Case 1: high-conductivity (“superconducting”) particles

For the case of high-conductivity particles (phase 2) in a lower-conductivity matrix (phase 1), we have:

$$1 \ll \frac{\sigma_2}{\sigma_1} \stackrel{\text{def}}{=} \alpha. \tag{6.1}$$

Inserting this expression into the Hashin–Shtrikman bounds and taking the limit as $\alpha \rightarrow \infty$ yields,

$$\sigma_1 \left(\frac{1 + 2\nu_2}{1 - \nu_2} \right) \stackrel{\text{def}}{=} \sigma_1 \zeta \leq \sigma^* \leq \infty, \tag{6.2}$$

where the lower (Hashin–Shtrikman) bound is more accurate ($\phi \rightarrow 0$). Correspondingly, for the concentration tensors for phase 1 (assuming isotropy)³

$$C_{E,1} = \frac{1}{1 - \nu_2} \quad \text{and} \quad C_{J,1} = \frac{1}{\zeta(1 - \nu_2)} = \frac{1}{1 + 2\nu_2} \tag{6.4}$$

and for phase 2 (particle)

$$C_{E,2} = 0 \quad \text{and} \quad C_{J,2} = \frac{1}{\nu_2} \left(1 - \frac{1}{\zeta} \right) = \frac{3}{1 + 2\nu_2}. \tag{6.5}$$

The expressions are appropriate for small ν_2 (superconducting particles in a binding matrix). For the various limiting criteria, we have:

- **Criterion #1:** In order to *not* exceed the electrical field strength for phase 1 (matrix):

$$\| \langle \mathbf{E} \rangle_\Omega \| \leq \frac{E_{1,crit}}{C_{E,1}} = E_{1,crit}(1 - \nu_2), \tag{6.6}$$

and for phase 2 (particle)

$$\| \langle \mathbf{E} \rangle_\Omega \| \leq \frac{E_{2,crit}}{C_{E,2}} = \infty. \tag{6.7}$$

- **Criterion # 2:** In order for the loading *not* to exceed the current field strength for phase 1 (matrix):

$$\| \langle \mathbf{J} \rangle_\Omega \| \leq \frac{J_{1,crit}}{C_{J,1}} = J_{1,crit}(1 + 2\nu_2), \tag{6.8}$$

and for phase 2 (particle)

$$\| \langle \mathbf{J} \rangle_\Omega \| \leq \frac{J_{2,crit}}{C_{J,2}} = J_{2,crit} \frac{(1 + 2\nu_2)}{3}. \tag{6.9}$$

- **Criterion # 3:** In order for the loading *not* to exceed the Joule-field strength for phase 1 (matrix)

$$\langle H \rangle_{\Omega_1} = \frac{\langle H \rangle_\Omega}{(1 - \nu_2)(1 + 2\nu_2)} \leq J_{1,crit} E_{1,crit} \Rightarrow \langle H \rangle_\Omega \leq J_{1,crit} E_{1,crit} (1 - \nu_2)(1 + 2\nu_2), \tag{6.10}$$

while for phase 2 (particle superconductor, no Joule-field)

$$\langle H \rangle_{\Omega_2} = 0. \tag{6.11}$$

As noted earlier, Criterion #3 results from the product of Criterion #1 and Criterion #2.

Remark. As $\nu_2 \rightarrow 0$ (no particle (phase 2) material), the expressions collapse to restrictions on the pure matrix (here, phase 1) material.

³ These expressions are consistent with the identities

$$\nu_1 C_{E,1} + \nu_2 C_{E,2} = 1 \quad \text{and} \quad \nu_1 C_{J,1} + \nu_2 C_{J,2} = 1. \tag{6.3}$$

6.2. Case 2: low-conductivity (“insulator”) particles

For the case of low-conductivity particles (phase 1) in a higher-conductivity matrix (phase 2), we have:

$$1 \gg \frac{\sigma_1}{\sigma_2} \stackrel{\text{def}}{=} \gamma. \quad (6.12)$$

Inserting this expression into the Hashin–Shtrikman bounds and taking the limit as $\gamma \rightarrow 0$ yields,

$$0 \leq \sigma^* \leq \sigma_2 \left(\frac{2\nu_2}{3 - \nu_2} \right) \stackrel{\text{def}}{=} \sigma_2 \lambda, \quad (6.13)$$

where the upper (Hashin–Shtrikman) bound is more accurate ($\phi \rightarrow 1$). Correspondingly, for the concentration tensors (as $\gamma \rightarrow \infty$), for phase 1 (particle)

$$C_{E,1} = \frac{1 - \lambda}{1 - \nu_2} = \frac{3}{3 - \nu_2} \quad \text{and} \quad C_{J,1} = 0 \quad (6.14)$$

and for phase 2 (matrix)

$$C_{E,2} = \frac{\lambda}{\nu_2} = \frac{2}{3 - \nu_2} \quad \text{and} \quad C_{J,2} = \frac{1}{\nu_2}. \quad (6.15)$$

The expressions are appropriate for large ν_2 (insulating particles in a binding matrix). For the various limiting criteria, we have:

- **Criterion #1:** In order to *not* exceed the electrical field strength for phase 1 (particle):

$$\|\langle \mathbf{E} \rangle_\Omega\| \leq \frac{E_{1,\text{crit}}}{C_{E,1}} = E_{1,\text{crit}} \frac{3 - \nu_2}{3}, \quad (6.16)$$

and for phase 2 (matrix)

$$\|\langle \mathbf{E} \rangle_\Omega\| \leq \frac{E_{2,\text{crit}}}{C_{E,2}} = E_{2,\text{crit}} \frac{3 - \nu_2}{2}. \quad (6.17)$$

- **Criterion # 2:** In order for the loading *not* to exceed the current field strength for phase 1 (particle)

$$\|\langle \mathbf{J} \rangle_\Omega\| \leq \frac{J_{1,\text{crit}}}{C_{J,1}} = \infty, \quad (6.18)$$

and for phase 2 (matrix)

$$\|\langle \mathbf{J} \rangle_\Omega\| \leq \frac{J_{2,\text{crit}}}{C_{J,2}} = J_{2,\text{crit}} \nu_2. \quad (6.19)$$

- **Criterion # 3:** In order for the loading *not* to exceed the Joule-field strength for phase 1 (particle insulator, no Joule-field)

$$\langle H \rangle_{\Omega_1} = 0, \quad (6.20)$$

and for phase 2 (matrix)

$$\langle H \rangle_{\Omega_2} = \frac{2\langle H \rangle_\Omega}{(3 - \nu_2)\nu_2} \leq J_{2,\text{crit}} E_{2,\text{crit}} \Rightarrow \langle H \rangle_\Omega \leq J_{2,\text{crit}} E_{2,\text{crit}} \frac{(3 - \nu_2)\nu_2}{2}. \quad (6.21)$$

Remark. As $\nu_2 \rightarrow 1$ (no particle (here, phase 1) material), the expressions collapse to restrictions on the pure matrix (here, phase 2) material.

7. Coated and multiphase materials

In some applications, (multiply) coated particles (Fig. 2) or multiphase materials are useful in electrical applications. In either case, the load level can be written as for N phases

$$\langle \mathbf{E} \rangle_\Omega = \frac{1}{|\Omega|} \left(\int_{\Omega_1} \mathbf{E} d\Omega + \int_{\Omega_2} \mathbf{E} d\Omega + \int_{\Omega_3} \mathbf{E} d\Omega + \cdots + \int_{\Omega_N} \mathbf{E} d\Omega \right) = \nu_1 \langle \mathbf{E} \rangle_{\Omega_1} + \nu_2 \langle \mathbf{E} \rangle_{\Omega_2} + \nu_3 \langle \mathbf{E} \rangle_{\Omega_3} + \cdots + \nu_N \langle \mathbf{E} \rangle_{\Omega_N} \quad (7.1)$$

and

$$\langle \mathbf{J} \rangle_\Omega = \frac{1}{|\Omega|} \left(\int_{\Omega_1} \mathbf{J} d\Omega + \int_{\Omega_2} \mathbf{J} d\Omega + \int_{\Omega_3} \mathbf{J} d\Omega + \cdots + \int_{\Omega_N} \mathbf{J} d\Omega \right) = \nu_1 \langle \mathbf{J} \rangle_{\Omega_1} + \nu_2 \langle \mathbf{J} \rangle_{\Omega_2} + \nu_3 \langle \mathbf{J} \rangle_{\Omega_3} + \cdots + \nu_N \langle \mathbf{J} \rangle_{\Omega_N} \quad (7.2)$$

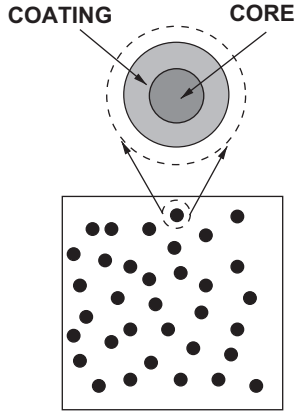


Fig. 2. A coated particle.

where $(v_1 + v_2 + v_3 + \dots + v_N = 1)$. Performing a set of straightforward algebraic manipulations yields

$$\begin{aligned}
 \langle \mathbf{J} \rangle_{\Omega} &= v_1 \langle \mathbf{J} \rangle_{\Omega_1} + v_2 \langle \mathbf{J} \rangle_{\Omega_2} + v_3 \langle \mathbf{J} \rangle_{\Omega_3} + \dots + v_N \langle \mathbf{J} \rangle_{\Omega_N} \\
 &= v_1 \boldsymbol{\sigma}_1 \cdot \langle \mathbf{E} \rangle_{\Omega_1} + v_2 \boldsymbol{\sigma}_2 \cdot \langle \mathbf{E} \rangle_{\Omega_2} + v_3 \boldsymbol{\sigma}_3 \cdot \langle \mathbf{E} \rangle_{\Omega_3} + \dots + v_N \boldsymbol{\sigma}_N \cdot \langle \mathbf{E} \rangle_{\Omega_N} \\
 &= \boldsymbol{\sigma}_1 \cdot (\langle \mathbf{E} \rangle_{\Omega} - v_2 \langle \mathbf{E} \rangle_{\Omega_2} - v_3 \langle \mathbf{E} \rangle_{\Omega_3} - \dots - v_N \langle \mathbf{E} \rangle_{\Omega_N}) \\
 &\quad + v_2 \boldsymbol{\sigma}_2 \cdot \langle \mathbf{E} \rangle_{\Omega_2} + v_3 \boldsymbol{\sigma}_3 \cdot \langle \mathbf{E} \rangle_{\Omega_3} + \dots + v_N \boldsymbol{\sigma}_N \cdot \langle \mathbf{E} \rangle_{\Omega_N} \\
 &= \underbrace{(\boldsymbol{\sigma}_1 + v_2(\boldsymbol{\sigma}_2 - \boldsymbol{\sigma}_1) \cdot \mathbf{C}_{E,2} + v_3(\boldsymbol{\sigma}_3 - \boldsymbol{\sigma}_1) \cdot \mathbf{C}_{E,3} + \dots + v_N(\boldsymbol{\sigma}_N - \boldsymbol{\sigma}_1) \cdot \mathbf{C}_{E,N})}_{\boldsymbol{\sigma}^*} \cdot \langle \mathbf{E} \rangle_{\Omega},
 \end{aligned} \tag{7.3}$$

where $\mathbf{C}_{E,i} \cdot \langle \mathbf{E} \rangle_{\Omega} = \langle \mathbf{E} \rangle_{\Omega_i}$, for $i = 2, 3, \dots, N$, given explicitly by

$$\mathbf{C}_{E,i} = \frac{(\boldsymbol{\sigma}_2 - \boldsymbol{\sigma}_1)^{-1}}{v_2} \cdot \left((\boldsymbol{\sigma}^* - \boldsymbol{\sigma}_1) - \sum_{j \neq 1, j \neq i} v_j (\boldsymbol{\sigma}_j - \boldsymbol{\sigma}_1) \cdot \mathbf{C}_{E,j} \right) \tag{7.4}$$

which leads to a coupled set of equations for the $\mathbf{C}_{E,i}$. For phase 1, since

$$\underbrace{v_1 \mathbf{C}_{E,1}}_{\text{phase-1 contribution}} + \underbrace{v_2 \mathbf{C}_{E,2}}_{\text{phase-2 contribution}} + \underbrace{v_3 \mathbf{C}_{E,3}}_{\text{phase-3 contribution}} + \dots + \underbrace{v_N \mathbf{C}_{E,N}}_{\text{phase-N contribution}} = \mathbf{1}. \tag{7.5}$$

therefore,

$$\mathbf{C}_{E,1} \stackrel{\text{def}}{=} \frac{1}{v_1} (\mathbf{1} - v_2 \mathbf{C}_{E,2} - v_3 \mathbf{C}_{E,3} - \dots - v_N \mathbf{C}_{E,N}) = \frac{\mathbf{1} - v_2 \mathbf{C}_{E,2} - v_3 \mathbf{C}_{E,3} - \dots - v_N \mathbf{C}_{E,N}}{1 - v_2 - v_3 - \dots - v_N} \tag{7.6}$$

where in the case of isotropy

$$\mathbf{C}_{E,1} = \frac{1 - v_2 C_{E,2} - v_3 C_{E,3} - \dots - v_N C_{E,N}}{1 - v_2 - v_3 - \dots - v_N} \tag{7.7}$$

For the current field, the concentration tensor for phase i

$$\mathbf{C}_{J,i} \cdot \langle \mathbf{J} \rangle_{\Omega} = \langle \mathbf{J} \rangle_{\Omega_i} \tag{7.8}$$

where $\mathbf{C}_{J,i} = \boldsymbol{\sigma}_i \cdot \mathbf{C}_{E,i} \cdot \boldsymbol{\sigma}_i^{-1}$. The Criteria #1 – #3 are still governed by Eqs. (4.1)–(4.8), with virtually no modification. *Once either the set of $\mathbf{C}_{E,i}$ or $\boldsymbol{\sigma}^*$ are known, the other can be determined.* However, sharp effective property bounds for N -phase composites are lacking in most cases, and one should probably resort to numerical discretization methods.

8. Summary and discussion

In principle, the approach introduced here can be used with other bounding or estimation techniques. To the knowledge of the author, Joule-field amplification estimates have not been previously investigated, although various bounds and estimates for other phase-wise fields can be found, for example, in the book of Kreher and Pompe [7]. The more general problem of estimating higher moments of the fields, in particular the second moments and the full distribution of the phase fields, can be found in Bergman [1], Cule and Torquato [2], as well as in a series of papers by Lipton, who explored local fields in depth (Lipton [11–14]). More detailed information, for example localized effects in the matrix ligaments between particles (“hot spots”), need to be generated numerically by solving a boundary-value problem posed over a statistically representative

volume element (RVE) sample of heterogeneous media. In particular, since time-transient effects lead to coupling of electrical and magnetic fields, the only viable approach is to employ direct numerical techniques to solve for Maxwell's equations. Specifically, one needs to solve Faraday's Law

$$\nabla \times \mathbf{E} = -\left(\frac{\partial \mathbf{B}}{\partial t} + \mathbf{M}_s + \mathbf{M}\right) \quad (8.1)$$

and Ampere's Law

$$\nabla \times \mathbf{H} = \frac{\partial \mathbf{D}}{\partial t} + \mathbf{J}_s + \mathbf{J} \quad (8.2)$$

where we recall that \mathbf{E} is the electric field, \mathbf{D} is the electric field flux, \mathbf{E} is the electric field, \mathbf{J} is the electric current, \mathbf{J}_s is the electric source current, \mathbf{H} is the magnetic field, \mathbf{B} is the magnetic field flux, \mathbf{M} is the equivalent magnetic current and \mathbf{M}_s is a phenomenological term that frequently appears in the literature to account for magnetic "sources/losses" and "magnetic conduction". Generally, these equations are strongly coupled. Additionally, if the local material properties are thermally-sensitive, and Joule-heating is significant, then the first law of thermodynamics must also be solved, simultaneously. Numerical techniques for the solution of coupled boundary-value problems posed over heterogeneous electromagnetic media, can be found in Zohdi [19], and are being developed further currently for such applications.

Appendix A. Averaging theorems

Two physically important (boundary) loading states that satisfy the micro-macro energy/power condition in Eq. (3.1). They are (1) pure electric fields of the form: $\mathbf{E}|_{\partial\Omega} = \mathcal{E} \Rightarrow \langle \mathbf{E} \rangle_{\Omega} = \mathcal{E}$ and (2) pure current field of the form: $\mathbf{J}|_{\partial\Omega} = \mathcal{J} \Rightarrow \langle \mathbf{J} \rangle_{\Omega} = \mathcal{J}$, where \mathcal{E} and \mathcal{J} are constant electric field and current field vectors, respectively. Clearly, for these loading states to be satisfied within a macroscopic body under nonuniform external loading, the sample must be large enough to possess small boundary field fluctuations relative to its size. Therefore, applying (1)- or (2)-type boundary conditions to a large sample is a way of reproducing approximately what may be occurring in a statistically representative microscopic sample of material within a macroscopic body. We record two classical results.

A.1. The average electric field theorem

We consider a body with $\mathbf{E}|_{\partial\Omega} = \mathcal{E}$. We make use of the identity

$$\nabla \times (\mathbf{E} \otimes \mathbf{x}) = (\nabla \times \mathbf{E}) \otimes \mathbf{x} + \underbrace{\mathbf{E} \cdot \nabla \mathbf{x}}_{\mathbf{E}} \quad (10.1)$$

and substitute this in the definition of the average electric field

$$\begin{aligned} \langle \mathbf{E} \rangle_{\Omega} &= \frac{1}{|\Omega|} \int_{\Omega} (\nabla \times (\mathbf{E} \otimes \mathbf{x}) - \underbrace{(\nabla \times \mathbf{E}) \otimes \mathbf{x}}_{=\mathbf{0}}) d\Omega = \frac{1}{|\Omega|} \int_{\partial\Omega} \mathbf{n} \times (\mathbf{E} \otimes \mathbf{x}) dA \\ &= \frac{1}{|\Omega|} \int_{\partial\Omega} \mathbf{n} \times (\mathcal{E} \otimes \mathbf{x}) dA = \frac{1}{|\Omega|} \left(\int_{\partial\Omega} (\nabla \times \mathcal{E}) \otimes \mathbf{x} d\Omega + \int_{\partial\Omega} \mathcal{E} \cdot \nabla \mathbf{x} d\Omega \right). \end{aligned} \quad (10.2)$$

Thus, if $\nabla \times \mathbf{E} = \mathbf{0}$, then $\langle \mathbf{E} \rangle_{\Omega} = \mathcal{E}$.

A.2. The average current theorem

We consider a body with $\mathbf{J}|_{\partial\Omega} = \mathcal{J}$. We make use of the identity

$$\nabla \cdot (\mathbf{J} \otimes \mathbf{x}) = (\nabla \cdot \mathbf{J}) \mathbf{x} + \underbrace{\mathbf{J} \cdot \nabla \mathbf{x}}_{\mathbf{J}} \quad (10.3)$$

and substitute this in the definition of the average current

$$\begin{aligned} \langle \mathbf{J} \rangle_{\Omega} &= \frac{1}{|\Omega|} \int_{\Omega} (\nabla \cdot (\mathbf{J} \otimes \mathbf{x}) - \underbrace{(\nabla \cdot \mathbf{J}) \mathbf{x}}_{=\mathbf{0}}) d\Omega = \frac{1}{|\Omega|} \int_{\partial\Omega} \mathbf{n} \cdot (\mathbf{J} \otimes \mathbf{x}) dA \\ &= \frac{1}{|\Omega|} \int_{\partial\Omega} \mathbf{n} \cdot (\mathcal{J} \otimes \mathbf{x}) dA = \frac{1}{|\Omega|} \left(\int_{\partial\Omega} (\nabla \cdot \mathcal{J}) \otimes \mathbf{x} d\Omega + \int_{\partial\Omega} \mathcal{J} \cdot \nabla \mathbf{x} d\Omega \right). \end{aligned} \quad (10.4)$$

Thus, if $\nabla \cdot \mathbf{J} = 0$, then $\langle \mathbf{J} \rangle_{\Omega} = \mathcal{J}$.

Appendix B. Basic thermodynamic relations

Joule-heating can be motivated by forming the inner product of the magnetic field with Faraday's law:

$$\mathbf{H} \cdot (\nabla \times \mathbf{E}) = -\mathbf{H} \cdot \left(\underbrace{\mathbf{M}_s + \mathbf{M}}_{\mathbf{M}^{tot}} + \frac{\partial \mathbf{B}}{\partial t} \right) \quad (11.1)$$

and the inner product of the electric field with Ampere's law:

$$\mathbf{E} \cdot (\nabla \times \mathbf{H}) = \mathbf{E} \cdot \left(\underbrace{\mathbf{J}_s + \mathbf{J}}_{\mathbf{J}^{tot}} + \frac{\partial \mathbf{D}}{\partial t} \right). \quad (11.2)$$

Subtracting Eq. (11.1) from Eq. (11.2) yields

$$\underbrace{\mathbf{E} \cdot (\nabla \times \mathbf{H}) - \mathbf{H} \cdot (\nabla \times \mathbf{E})}_{-\nabla \cdot (\mathbf{E} \times \mathbf{H}) = -\nabla \cdot \mathbf{S}} = \mathbf{E} \cdot \mathbf{J}^{tot} + \mathbf{H} \cdot \mathbf{M}^{tot} + \underbrace{\mathbf{E} \cdot \frac{\partial \mathbf{D}}{\partial t} + \mathbf{H} \cdot \frac{\partial \mathbf{B}}{\partial t}}_{=\frac{\partial W}{\partial t}}, \quad (11.3)$$

where $W = \frac{1}{2}(\mathbf{E} \cdot \mathbf{D} + \mathbf{H} \cdot \mathbf{B}) = \frac{1}{2}(\mathbf{E} \cdot \boldsymbol{\epsilon} \cdot \mathbf{E} + \mathbf{H} \cdot \boldsymbol{\mu} \cdot \mathbf{H})$ is the electromagnetic energy and where $\mathbf{S} = \mathbf{E} \times \mathbf{H}$ is the Poynting vector. Thus

$$\frac{\partial W}{\partial t} + \nabla \cdot \mathbf{S} = -(\mathbf{E} \cdot \mathbf{J}^{tot} + \mathbf{H} \cdot \mathbf{M}^{tot}), \quad (11.4)$$

Eq. (11.4) is usually referred to as Poynting's theorem. This can be interpreted, *for simple material laws, where the previous representation for W holds*, as stating that the rate of change of electromagnetic energy within a volume, plus the energy flowing out through a boundary, is equal to the negative of the total work done by the fields on the sources and conduction. This work is then converted into thermo-mechanical energy ("Joule-heating", H in Eq. (1.2)). On the sub-continuum scale, Joule-heating arises from charged particles being pulled through a medium by electromagnetic fields, which generate heat when they collide with the surrounding medium.

Appendix C. Special cases of Maxwell's equations

By taking the divergence of Ampere's law:

$$\nabla \cdot \left(\nabla \times \mathbf{H} - \frac{\partial \mathbf{D}}{\partial t} - \mathbf{J}_s - \mathbf{J} \right) = 0, \quad (12.1)$$

one obtains, since

$$\nabla \cdot (\nabla \times \mathbf{H}) = 0, \quad (12.2)$$

$$\nabla \cdot \left(\frac{\partial \mathbf{D}}{\partial t} + \mathbf{J}_s + \mathbf{J} \right) = 0, \quad (12.3)$$

thus

$$\frac{\partial}{\partial t} \underbrace{\nabla \cdot \mathbf{D}}_{\mathcal{P}} + \nabla \cdot (\mathbf{J}_s + \mathbf{J}) = 0, \quad (12.4)$$

thus

$$\frac{\partial \mathcal{P}}{\partial t} + \nabla \cdot (\mathbf{J}_s + \mathbf{J}) = 0. \quad (12.5)$$

Thus, if $\mathcal{P} = 0$ and $\nabla \cdot \mathbf{J}_s = 0$,

$$\nabla \cdot \mathbf{J} = 0. \quad (12.6)$$

If one employs the constitutive relation $\mathbf{J} = \boldsymbol{\sigma} \cdot \mathbf{E}$, then this allows for Hashin–Shtrikman type estimates for effective conductivity, as does the PDE $\nabla \cdot \mathbf{D} = 0$ (which is valid only then $\mathcal{P} = 0$) for the effective permittivity, $\langle \mathbf{D} \rangle_{\Omega} = \boldsymbol{\epsilon}^* \cdot \langle \mathbf{E} \rangle_{\Omega}$, when $\mathbf{D} = \boldsymbol{\epsilon} \cdot \mathbf{E}$. For example, one case when these two physical situations are compatible is when

$$\mathbf{E} = \boldsymbol{\sigma}^{-1} \cdot \mathbf{J} = \boldsymbol{\epsilon}^{-1} \cdot \mathbf{D} \Rightarrow \mathbf{J} = (\boldsymbol{\sigma} \cdot \boldsymbol{\epsilon}^{-1}) \cdot \mathbf{D}. \quad (12.7)$$

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