1 Effective Medium Approximations

In the sample structure, a mixed phase material material may be specified using the format

$$[\ \{\text{model}\}\ \ f_1\ \ mat_A\ \ f_2\ \ mat_B\ \ \ldots\ ]$$

where the EMA (Effective Medium Approximation) model may be optionally specified followed by volume fractions of various materials. The sum $f_A + f_B + \ldots$ need not be unity as TFOC will normalize the values. Each of the materials mat_i may either be a specific material from the database or may itself be a mixed phase model.

Some specific examples are

- [0.8 Si 0.2 SiO2] 30
- [PARALLEL 0.3 Si 0.4 Si3N4 0.3 SiO2] 120
- [0.8 Si 0.1 [0.3 SiO2 0.7 Si3N4] 0.1 Al2O3] 80
- [LOOYENGA 0.8 Si 0.1 [BRUGGEMAN 0.3 SiO2 0.7 Si3N4] 0.1 Al2O3] 250

The code implements sevearl EMA models which are strictly valid in specific sample constructs.

- **Series (default):** The series mixing is a simple weighted sum of the dielectric constants of the elements. This model is symmetric and valid for any number of components.

$$\epsilon_{\text{eff}} \quad = \quad \sum f_i \epsilon_i$$

- **Parallel:** The parallel model is the other limit for the dielectric constant of an arbitrary mixture. Like the series model, it is valid for an arbitrary number of components and is symmetric in all components:

$$\frac{1}{\epsilon_{\text{eff}}} \quad = \quad \sum \frac{f_i}{\epsilon_i}$$

- **Looyenga:** This model uses a weighted sum of the dielectric constant to the 1/3 power. See H. Looyenga, *Dielectric constants of heterogeneous mixtures*, Physica **31**, 401-406 (1965). Again, like the previous two, it has the advantage of being extensible to multiple components and all phases are treated symmetrically.

- **Bruggeman:** Bruggeman in the 1930's created the master of all EMAs. The form is deceptively simple and symmetric in any number of components, but as it does not have a closed form solution it is implemented for only two components in the code. The model is based on the equation:

$$\sum f_i \frac{\epsilon_i - \epsilon_{\text{eff}}}{\epsilon_i + (n-1)\epsilon_{\text{eff}}} = 0$$

  where n is the dimensionality of the mixture (3 for normal 3D). For two terms, ϵ_{eff} can be written as

$$\epsilon_{\text{eff}} \quad = \quad \frac{\epsilon_A(3f_A - 1) + \epsilon_B(2 - 3f_A) + \sqrt{[\epsilon_A(3f_A - 1) + \epsilon_B(2 - 3f_A)]^2 + 8\epsilon_A\epsilon_B}}{4}$$

- **Maxwell-Garnett:** This EMA was derived to explain the color in glasses and is valid primarily in the low volume fraction limit where the inclusions do not interact. The lower volume fraction component is taken as the inclusion (ϵ_i) while the majority component is the matrix (ϵ_m). This model is implemented for only two components and is not symmetric in the two elements. The equation takes the form:

$$\begin{aligned} \frac{\epsilon_{\text{eff}} - \epsilon_m}{\epsilon_{\text{eff}} + 2\epsilon_m} \quad &= \quad f_i \left(\frac{\epsilon_i - \epsilon_m}{\epsilon_i + 2\epsilon_m} \right) \\ \epsilon_{\text{eff}} \quad &= \quad \left[\frac{\epsilon_i(1 + 2f_i) - \epsilon_m(2f_i - 2)}{\epsilon_m(2 + f_i) + \epsilon_i(1 - f_i)} \right] \epsilon_m \end{aligned}$$

The models are derived for pure dielectrics. TFOC blindly extends these to the complex dielectric constant and uses $n = \sqrt{\epsilon}$. There is discussion of limits for complex dielectric constants which may later be implemented:

References:

1. D.A. Bruggeman, Annalen der Physik, **24** (1933), 636-664.
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3. D.J Bergman, Phys. Rev. Lett. **44** (1980), 1285-1287.
4. G.W. Milton, Appl. Phys. Lett. **37** (1980), 300-302.