Property and Performance Prediction of Meta Composites for Novel Applications

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Abstract: Metacomposites are new class of materials engineered for unusual properties. The focus of this paper is on the modeling methods for predicting the effective properties and performance of metacomposites for novel application development. Numerical models in COMSOL were developed to investigate the macro behavior using homogenized macro and heterogeneous microstructure based models. Computer aided Micro Mechanical models leverage the actual micro structure to predict the macro performance. The homogenized model uses the effective properties for macro performance evaluation of metacomposites. The macro micro modeling method provides many benefits for metacomposites performance evaluation at the cost of complexity, time and resources. The micro mechanical model allows engineering the constituents to get the desired effective properties. The details of the model development, the simulation method and results are reported. The performance prediction method and its applications related to flat lens, cloaking ing, engineered wave propagation, high impedance surfaces, antenna miniaturization and super lens are highlighted for both electromagnetic and acoustics meta materials.

Keywords: meta material, meta composites, micro mechanics, homogeneous, Computer aided micromechanics, multilevel models, engineered composites, material design.

1. Introduction

Metacomposites are new class of materials with unusual properties that can be engineered using existing materials for usual properties [1-16]. The unusual properties of metacomposites are derived from the structure, analogues to atomic arrangement in crystal lattice. These material exhibits unusual behavior to electromagnetic wave propagation and thus enables novel applications. Metamaterials provide an opportunity to engineer the existing materials for unusual properties that does not exist in nature for novel engineering applications. The developments in metamaterials are at fundamental physics level and hence can institute completely new engineering field. The degree of freedom available at atomic level is so large and was exploited for synthesis of large compounds and materials. Metamaterials enables one step above to arrange the periodicity of materials for unusual material property by engineering the arrangement for novel properties

A multilevel macro micro modeling method leveraging macro behavior using homogenized macro and heterogeneous microstructure based models is developed. A multilevel modeling methodology for meta material application development with effective properties and engineering microstructure to get the effective properties are detailed. A comparison of performance prediction using micromechanical and homogenized properties based models are also shown. The formulation and model development in COMSOL are detailed. The wave propagation results predicted for micromechanical and homogenized models are shown. Comparison of results highlights the effectiveness of modeling method in performance prediction for novel applications. The micromechanical models results are shows for the elastic resonance and permittivity of metacomposites. A Multi-level modeling approach and its benefits for novel metacomposites application development by combining micromechanics and effective property prediction simulation methods are highlighted.

2. Metamaterials

Victor Vesalago [1] proposed in his 1968 seminal paper on negative materials and the possibility of having negative electrical permittivity and magnetic permeability for novel applications. The concept has also been explored by other researchers on various contexts from earlier times. However, the recent exponential growth is spurted after the experimental demonstration of these concepts in a laboratory [3.12]. Meta composites are the periodic arrangement of dissimilar materials. The wave interaction with dissimilar materials can provide superior or unusual properties. Waves can have, go or no go conditions to provide band gaps such as electromagnetic band gaps, photonic band gaps and phononic band gaps, depending on the type of wave and interactions.

The novel metamaterial based applications explored by other researchers [1-3, 12-16], include, Radio Frequency/ Microwave Passive Components, Electromagnetic bang gap based Imaging, Small and or Planar Antennas, Antenna Beam forming, Cloaking, Stealth materials, Medical Imaging, Flat lens focusing, Tunable and Active materials, EMI Reduction or shielding, 100% solar Absorbing, Graded Porous Thermal barrier coatings, Room Temperature Superconductors, 100 % sound proof walls, Quantum Levitation, Wireless Power Transfer, 100% efficient Antireflective structures, metasurfaces and more. The meta material conceptual illustration on the permeability and permittivity space with typical class of metamaterials is shown in figure 1.

The fundamental physics properties related to these applications include Interference, Diffraction, Absorption, Scattering, Polarization, Dispersion, Reflection, Refraction, and Transmission. These materials are targeted for breakthroughs in energy harvesting, miniaturization of communication antenna, medical and security imaging, and defence stealth applications. The critical destructive interference, constructive interference and scattering effects are shown in figure 2.

Concept of metamaterials expands beyond electromagnetics [7]. The exploration of acoustics waves for metamaterial effects lead to the growth of acoustics metamaterials [3]. Acoustics meta material is analogues to magnetic meta material, where in density and elastic stiffness, wave propagation parameters are engineered for unusual properties. Acoustic metamaterials research can be summarized as, Sonic at 1-20kHz frequency range with wave length in 'm' range for Sound engineering applications, Ultrasonic at 20kHz-1GHz frequency range with wave length in 'mm' range for imaging and Nondestructive Evaluation and Hypersonic with a frequency greater than 1GHz range and wave length in 'um' range for thermoelectric, and acoustic-optical coupling applications. The acoustic imaging beyond the diffraction limit and acoustic cloaking ing are critical acoustics applications under development. The metamaterial concept is also further explored by other researchers for mechanical and elastic waves for unusual applications.

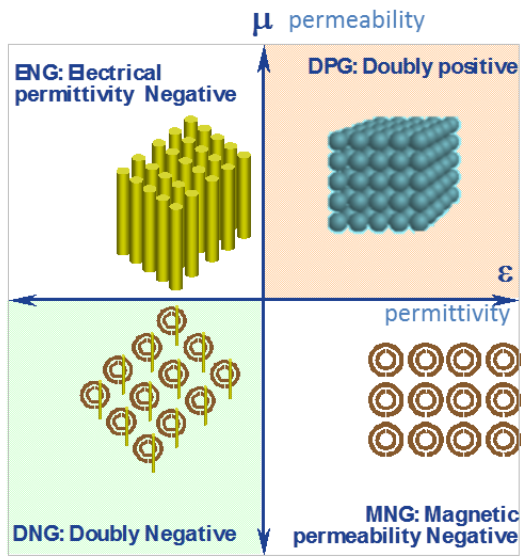
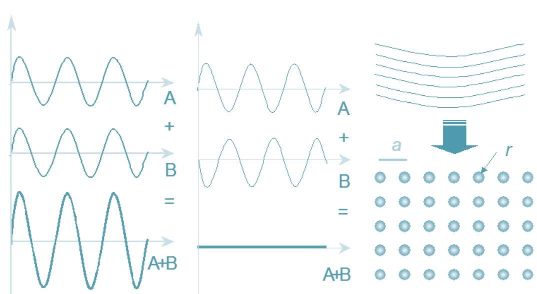


Figure 1 Illustration of metamaterial on permittivity and permeability space with typical applications.



(a) (b) (c)

Figure 2 Illustration of wave propagation effects (a) constructive interference, (b) destructive interference and (c) scattering effects

The advantages of metamaterial projected are material with unusual, super and extreme properties for Novel Applications in the entire electromagnetic spectrum. This spectrum covers a wide range, and the modeling to application conversion is taking place from Radio waves towards X-rays due to limitations in the manufacturing capability. The fabrication methods used are conventional fabrication methods that are extended for metamaterial fabrication. The challenges are the dispersive nature of metamaterials, the narrow bandwidth, and resonant behaviors. The Absorption, loss less medium seems to significant which influence the figure of merit. Homogenization and effect of tolerance are under active research. The ways to make 3D metamaterials with isotropic properties are of concerns raised by the researchers.

A basic element of metamaterial design is a unitcell of identical building blocks, like the crystal lattice. These unit cell interaction with electromagnetic, acoustics or other waves manifests into macro performance with unusual properties. The wave interaction effects with the unit cell are critical and the constituents of the unitcell can be engineered to interact for unusual properties. The wave propagation inside the material is due to effective interaction of wave with the constituents, when waves move through the material they respond to the material as a whole, as if it were a homogeneous substance. This behavior is leveraged in two step process for novel application development by, first macro application development with effective properties and secondly engineering constituents for effective property. The optimization methodology available in COSMOL can also be leveraged for finding the optimal constituent configuration and properties as an inverse material design problem.

3. Micromechanics of Metacomposites

Metamaterials facilitate developments of new material with unusual electromagnetic properties by engineering the existing materials. Similarly, thermal, electrical, magnetic, transport, optical and acoustic composite materials are under development for unusual and superior specific properties [3,7,12]. Composite definition based on specific morphology or length scale can be defined as materials which is homogeneous at 'n+1' length scale and heterogeneous at 'n' length scale. Usually, n+1 length scale refers to macro and 'n' length scale refers to 'n' micro and n-1 length scale refers to nano length scale. This broader definition can encompass atomic to nano to macro to meta composites. Multiscale windowing approach leveraging multilevel model can be used for engineered material based on application development requirement [10].

The benefits of computer aided micro mechanics are virtual cost effective new product development, reduction in actual experimentation, faster product development, numerical scanning of suitable fillers, and virtual optimization for multiple properties [11]. Conventional experimentation based methods do not leverage the essential physics of composites for simulation based material development. The advantages of computer-aided micromechanics [6,8] are rooted in physics based model from atomic to molecular level. This methodology enables to design new material system with unusual, novel and superior properties by leveraging existing materials, as synthesis of new materials are relatively expensive.

In order to develop unique material, we need to engineer constituent properties, interface behavior, and the microstructure or morphology. The macro properties are emerging from the constituent property and interaction. The response of a composite structure initiates from atomic level to molecular to morphology to constituents to macro properties. Tailoring these parameters through simulations can help to design material with better properties by factoring the constituent effects and interaction. The multilevel modeling mythology can enable digital design of filler based materials. The schematic illustration of multilevel modeling of computer-aided micromechanics for meta material development is shown in figure 3.

Inverse material design is another material design opportunity, which helps to design materials to solve for a specific industrial problem. Exploration of microstructure or morphology by experiments alone will take more time. The virtual exploration is a successful approach for faster material design beyond the experimental limitation.

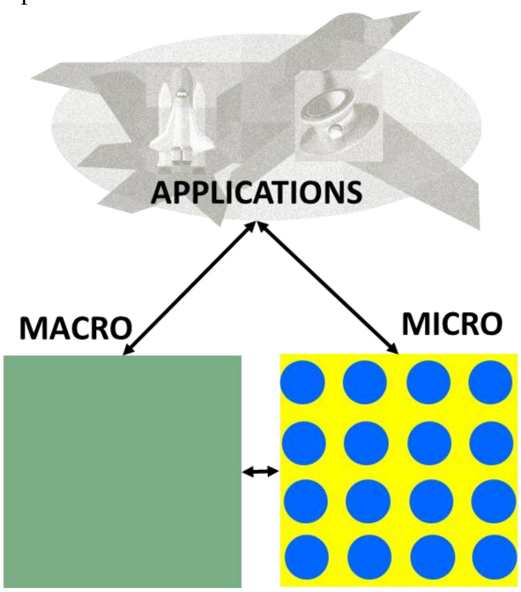


Figure 3. Schematic illustration multilevel modeling methodology for metamaterial based application development with effective macro and constituent micro models.

The representative volume elements with CAD models and microstructure help to model realistic material morphology for property prediction. A windowing approach is explored for designing metamaterial by combining macro (n+1 level) equivalent property prediction and micro (n level) effective property prediction. The methodology adopted from composite material mechanics design for Meta material is detailed. The simulation results are presented for both analytical and computer aided micromechanical models. The modeling methodology is expected accelerate metamaterial based application development. As the micro structure and homogenized model can be leveraged for product development. The implementation of the model development in COMSOL [5] is detailed in the next section.

4. Numerical Model development

In this paper the electromagnetic and acoustics meta materials are considered. Hence, the governing equation related to electromagnetic and acoustics simulations are given below. The following two Maxwell equations govenrns the interaction of eletromagnetic field with materials and relate the time varations of one field to spatial variation of the other.

$$\overline{\nabla}\text{x}\ \overline{\text{H}} = \sigma\overline{E} + \varepsilon\frac{\partial\overline{E}}{\partial t}$$

$$\overline{\nabla}\text{x}\ \overline{\text{E}} = -\mu\frac{\partial\overline{H}}{\partial t}$$

Where,

$\overline{\text{E}}$, electric field vector,

$\overline{\text{H}}$, magnetic field vector,

σ, conductivity,

ε, permittivity,

μ, permeability.

Maxwell's equation reduced into the wave equation, is used for wave propagation investigations in this paper, as given below,

$$\left(\nabla^2 - \frac{n^2}{c^2}\frac{\partial^2}{\partial t^2}\right)\psi = 0$$

Where, n is refractive index, c is the velocity of light in vacuum and $(n^2/c^2) = \varepsilon\mu$. Further, ε refers to the electrical permittivity and μ refers to the magnetic permeability. Frequency dependent Electromagnetic properties are of focus and hence the COMSOL's electromagnetic interface with frequency domain [5] is used for electromagnetic metamaterial simulations.

The acoustics wave propagation in the medium is handled by the wave propagation equation. Acoustic waves in a lossless medium are governed by the following inhomogeneous Helmholtz equation.

$$\frac{1}{\rho_0 c_s^2}\frac{\partial^2 p}{\partial t^2} + \nabla.\left(-\frac{1}{\rho_0}(\nabla p - \text{q})\right) = Q$$

Where, ρ_0 in kg/m^3, refers to the density and c_s in m/s is the speed of sound, p *in* (N/m^2), is the differential pressure and Q *in* $1/s^2$ is the source. The pressure acoustics interface in COMSOL [5] is used for acoustical wave propagation simulations for acoustical metamaterial applications.

COMSOL model with appropriate material properties, boundary conditions and mesh parameters were used for performance. The constituent material properties and effective properties of unitcell models were also validated. The wave propagation contour plots and integration features were used to estimate and compare the overall performance. The frequency dependent effects were also considered. For Electromagnetic performance optical frequency range and acoustical performance ultrasonic frequency range was considered.

5. Results and Discussion

The electromagnetic wave propagation in composite medium, negative refraction, electrostatic resonance and composite cloaking ing effects are described in this section. The acoustic metamaterial based super lens concept simulation results are also highlighted. The homogeneous effective property based simulation is compared with micromechanical constituent property based simulation. The multilevel simulation concept results are illustrated in figure 4. The figure shows results for a negative refractive index medium of -1 sandwiched between regular medium with refractive index of 1. Identical performance was observed for both homogeneous and heterogeneous medium based simulations.

The effective permittivity prediction and wave propagation in conventional medium with equivalent effective permittivity of 1.95 is shown in figure 5. Figure 6 shows the wave propagation performance for similar systems with constituent micro mechanical property and configuration. The medium was modeled with constituent microstructure morphology and properties to provide effective permittivity of 1.95. An air and polymer mixture was used to get the effective permittivity leveraging the available material by micro mechanical simulations. Figures 5 and 6, contour plot shows almost identical wave propagation performance. The transmission performance was also compared. This shows that the permittivity of the composite calculated from the proposed methodology precisely predicts the effective permittivity of the homogenous medium, thus confirming the effectiveness of effective property prediction methodology using Computer Aided Micro-Mechanics.

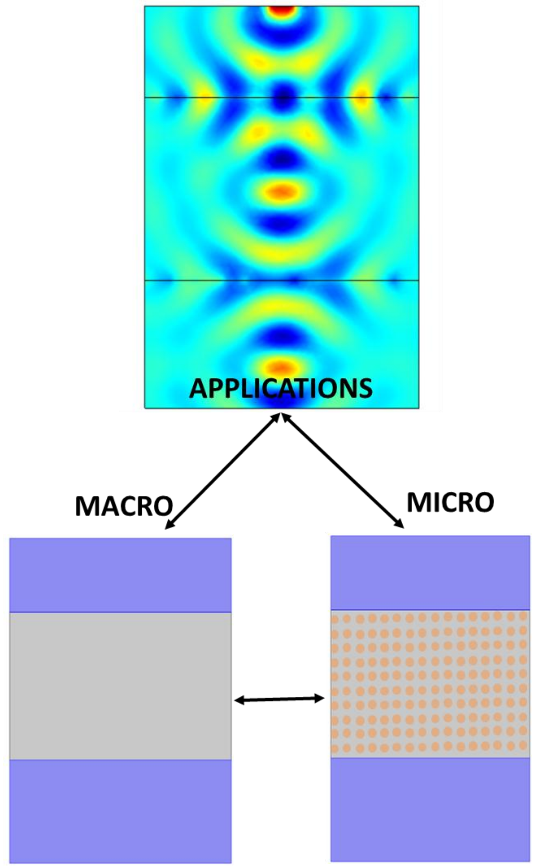


Figure 4 shows typical electromagnetic super lens simulation results for macro effective property and micro constituent property based performance evaluation.

Figure 7 shows the negative refraction simulation results for constituent property based modeling. The constituents, air and polymer matrix were engineered to provide super lens effect with effective negative properties. Figure 7 shows the focusing effect with ultrasonic metamaterials. Similar results were also observed with effective properties. Thus the modeling method shows that the overall performance for novel application can be explored numerically by assuming an effective property. The constituents to get the effective properties can then be searched through micro mechanical models. The constituent geometry and properties can also be used as an input to limit the design space. The inverse material design method can be used for engineering novel morphology.

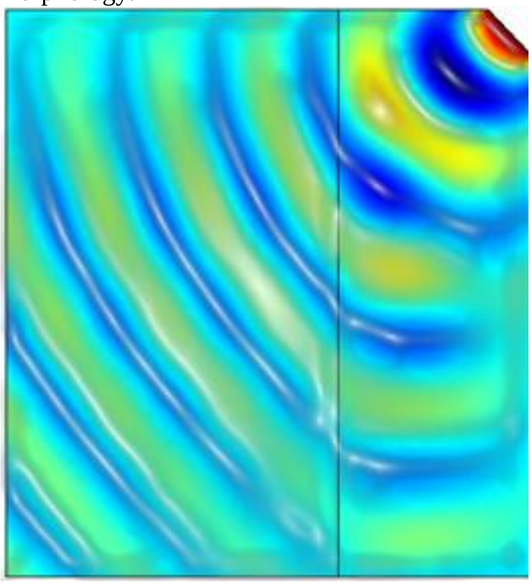


Figure 5 Contour plots of wave propagation through the metacomposites with homogenized medium with effective properties

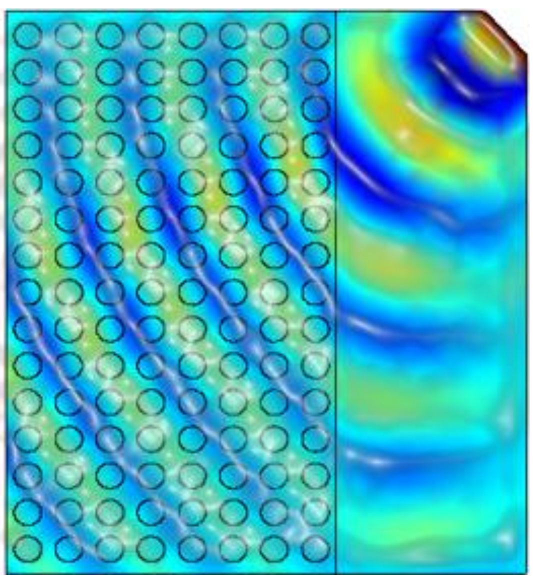


Figure 6 Contour plots of wave propagation through the composite medium with heterogeneous microstructure with explicit constituent and properties.

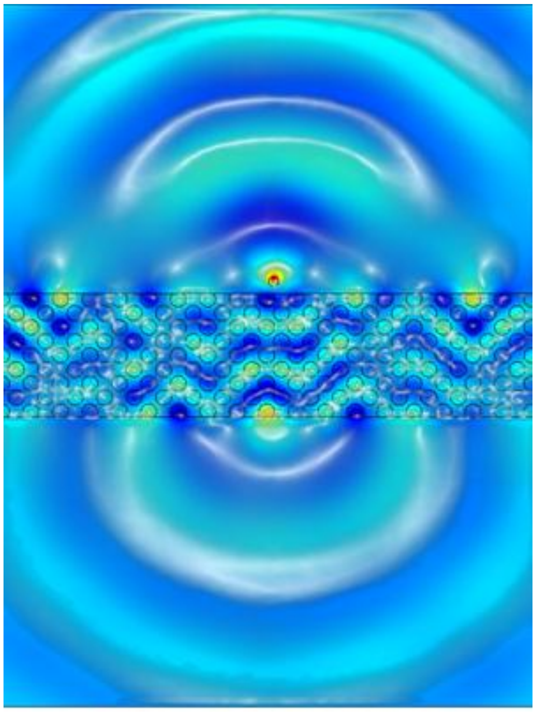


Figure 7 Illustration of acoustical meta material demonstrating super lensing behavior using metacomposites.

6. Conclusions

An overview of the meta materials developments was given. The unusual properties of interest related to meta materials and target applications of interest are detailed. The brief overview of electromagnetic meta materials and acoustic meta materials was given. The metamaterials in the permittivity and permeability space, interference and scattering effects are highlighted. An overview of computer aided micro mechanical models was given. The multilevel modeling methodology to predict the performance with homogenous effective property and with heterogeneous microstructure based models was detailed. The numerical modeling and implementation in COMSOL were detailed with appropriate electromagnetic and acoustics wave propagation governing equations. A brief about boundary conditions, material properties are also given. The simulation results related to the multilevel modeling method for novel application development was highlighted. The results related to identical wave propagation in effective property based medium and constituent property based medium were detailed. The effectiveness of effective property prediction methodology was demonstrated with permittivity for wave propagation inside a homogenous and heterogeneous medium. Similar performance was demonstrated for acoustical super lens.

The focus of this paper was show the acceleration potential for novel meta material based application development leveraging the effective property based application and material development by multilevel models. The frequency dispersion, three dimensional effects, large volume manufacturing methods and experimental demonstration are under development.

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