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SUMMARY REPORT

Design and implementation of absorbing materials with a hybrid model based on multiscale modeling and machine learning-AIStealth

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Abstract
Protecting objects from sensors requires the development of new thin, lightweight, and more efficient broadband microwave absorption materials and structures. Traditional material development work based on experimental work is often time and labor consuming especially in applications having large amount of design parameters. Computational tools are one option to accelerate experimental material development. In recent years, coarser models based on machine learning have also been introduced, which enable faster prediction of material properties by calculation. As a result of the project, computational tools were created for the systematic design of radar absorbing materials and structures, which the Defense Forces can utilize in both normal and crisis times, thus strengthening military security of supply.

1. Introduction

Electromagnetic spectrum control has been found to be an essential prerequisite in modern warfare. The rapid development of sensor systems has created the need to rapidly develop new methods for stimulus control as well. Controlling the excitations of the object's electromagnetic spectrum, and thereby securing performance, requires the development of new, more efficient absorption materials and structures. The need is emphasized in weight-critical objects, such as flying equipment (e.g.UAVs / payloads) as well as objects with a large surface area, such as ships and various mast structures. Protecting objects requires the development of new thin, lightweight, and more efficient broadband microwave absorption materials and structures. In previous development projects for absorber materials performance has reach the level where further improvement for absorption efficiency and weight reduction is not reasonable by traditional experimental work approach. The current performance has been achieved as a result of several years of development work and a significant amount of measurement data has been collected during it. Modelling assisted material development is one solution to minimize time and labour consuming experimental work. The focus of the development work has been on the development of multiscale models; in recent years, coarser models based on machine learning have also been introduced, which enable faster prediction of material properties by calculation. By combining an experimental and a computational approach, completely new solutions for excitation management can be developed: the experimental data collected so far provide a good basis for utilizing artificial intelligence and multiscale modeling in material development.

2. Research objectives and accomplishment plan

The overall goal of the project was to develop computational tools to accelerate experimental material development. The models developed are aiming a better understanding of the interactions between the absorber material and the microwave radiation, which enables the systematic development of new types of materials to meet the requirements of the application in question. The design problem of the Radar Absorbing Material (RAM) can be described following. A typical RAM solution consists of several layers that require different types of electrical and magnetic properties. Each layer (n) has a specific frequency-dependent complex electrical permittivity ϵ_n^* and a magnetic permeability μ_n^* as well as a density. The thickness of a layer is determined by both the material properties of that layer and the properties of the adjacent layers. The total structure is determined by the desired absorption level and frequency range. The single layer typically consists of a polymer matrix with certain electrical and magnetic (ϵ_m^* and μ_m^*) properties and further density ρ_m and volume fraction f_m. The properties of the polymer matrix are enhanced and adjusted to the desired level by various filler additions. Each active ingredient and filler have specific electrical and magnetic properties (ϵ_n^* and μ_n^*), respectively, as well as a density ρ_n, a shape / size factor S_n, an anisotropy factor A_n and a volume fraction f_n. Many types of micro-geometry related indictors can also be utilized. Even looking at a simple structure consisting of two layers, each with two different active ingredients / fillers, it can be noticed that the number of design parameters is large (18 variables) and thus the number of possible combinations is huge. Beside this is the fact that almost all parameters interact with each other, it can be said that finding the optimal solution experimentally (or even utilizing statistical experimental design methods) is very challenging and time consuming. The key question guiding the research was how the formation of the microstructure creating specific electrical and magnetic properties for absorber material can be modeled with sufficient accuracy and further how optimal solutions can be found from a large amount of design parameters. Other key question was how to measure/determine electromagnetic properties of filler material itself, especially in case of different shapes. As a result of the project, computational tools were created for the systematic design of radar absorbing materials and structures, which the Defense Forces can utilize in both normal and crisis times, thus strengthening military security of supply.

3. Materials and methods

The underlying research philosophy is based on the PSPP (Process - Structure -Property - Performance) framework explained in Fig. 1.

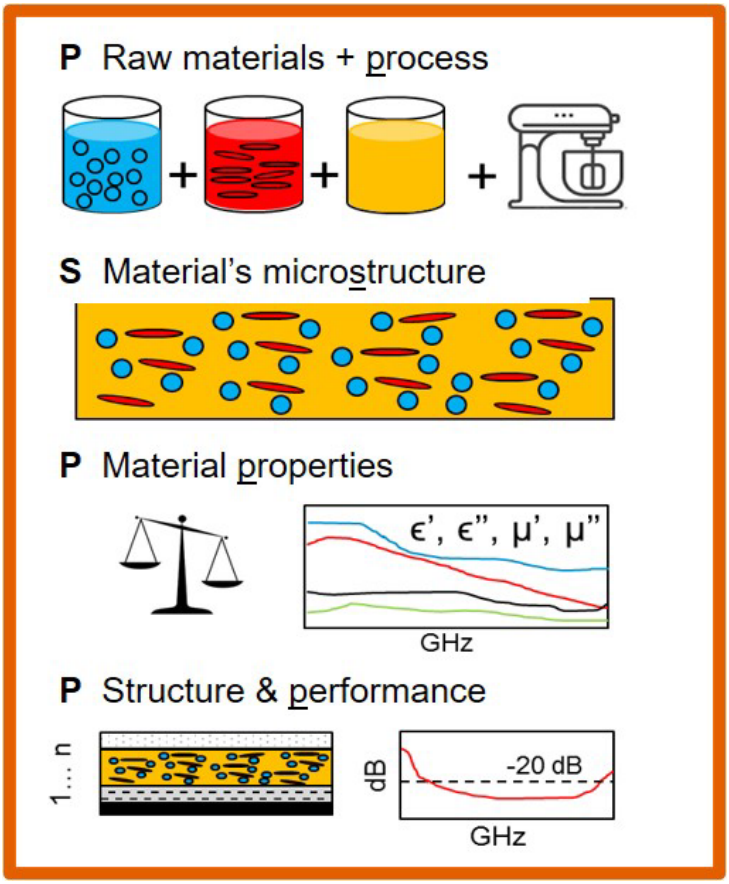

Fig.1. The four quadrants signify the following elements in PSPP research framework. Top left: P = Process (raw materials and sample preparation). Top right: S = Structure (microstructure analysis). Bottom left: P = Properties (measurement on sample's electro-magnetic response functions = permeability and permittivity). Bottom right: P = Performance (evaluation of the sample/product performance under conditions of interest).

At the beginning of the project to support the computational approach a systematic series of samples with selected active ingredients and filling factor were prepared and their material parameters ϵ* and μ* were measured. The microstructures were determined from the samples and the electromagnetic properties were measured. Alongside the new samples, samples and measurement data from previous projects were utilized when relevant. Experimental data was collected into the databank in the same format. Measured properties were obtained from the composite structure (filler particles + matrix).

To get the real electromagnetic properties of filler material alone, classical mixing formulas were screened and the best fits were selected to be able to calculate the filler material properties. After obtaining the effective permittivity and permeability spectra of the individual filler particle species from the composite specimen (reverse engineering), the results were utilized in EM response calculation of response spectra of new types of composites (which were not manufactured in laboratory). Different types of

optimization procedures can be applied to extract the best-fit permittivity and permeability properties of the filler material particles in addition to other design parameters obtainable from the statistical microstructure characterization.

Three different analytic and numerical methods were applied to derive and cast the numerical simulation model into an effectively computable form. The most accurate and slowest of the solution methods is the so-called full-field computation, which solves directly the electro-magnetic field equations for a given microstructure. Since the computation time depends on the system size, the numerical burden becomes very large for any realistic distribution of small-sized filler particles with possibly arbitrary shapes. In addition, the results must be averaged over the micro-geometry distributions. Due to the system size dependence and averaging requirements, the full-field method was deemed suitable only for calibration type exercises and replaced by faster surrogate methods.

Several types of faster to compute surrogates were developed. These can be divided into two groups. Surrogate model group A (semi-analytic surrogates) is characterized by models, whose structure is analytic with numerically solvable quadrature and extremizable parameters. In layman terms, one can say that these models provide permeability and permittivity as a complicated but explicit function of filler properties and micro-geometry parameters. Surrogate model type B was derived from group A by replacing certain quadratures (multiple nested integral expressions) with a black-box function generated by machine learning methods. Again, several teaching techniques can be applied, the best performing one in this case turned out to be gradient boosted trees method. In other words, some complicated integral expressions in type A models were replaced with an approximation (accurate enough and very fast to compute) obtained by supervised machine learning with the values of the slow quadrature expression as target values for teaching process. The reason why both types of surrogates A and B are substantially faster than the full electro-magnetic field based solutions derive from the fact that the microgeometry averaging has already been performed in the former and extrapolation of large system size is easier to perform. On the other hand, the disadvantage of the surrogate solutions is that we have to rely on simple geometrical forms for the filler particles such as rotation symmetric ellipsoids. In reality, the fillers have more irregular shapes. This observation, while restrictive, opens up additional possibilities for new types of statistical mechanics studies or more irregular types micro-geometry constituents to be described in Sect. 5.

4. Results and discussion

This work combines numerous results from three different fields. (1) First of all, several types of filler materials were produced and processed into a variety of shapes, which were embedded into two different types of matrices. The electromagnetic response functions (permittivities and permeabilities) of the matrix+filler composite were measured over a wide range of frequencies in the microwave region and stored in a database. This collection of data formed basis for the predictive modeling part. Additionally, interesting data was also obtained from the angle distribution of the filler particles based on analysis of SEM images in Fig.2.

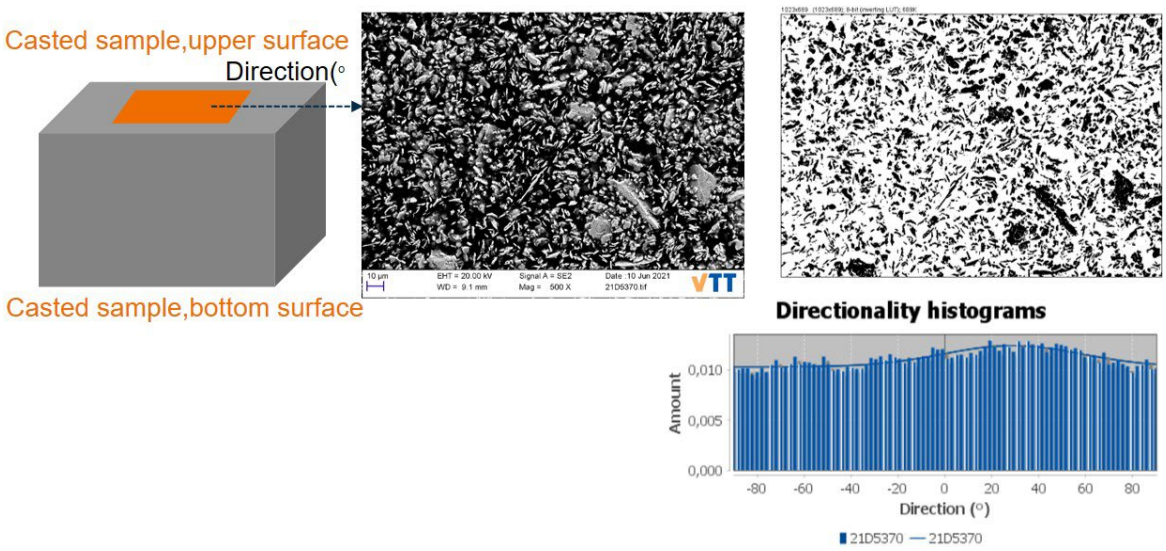

Fig.2 Scanning electron microscope pictures of the cross-section of a cast sample. Suitable filtered and manipulated measurement data was subjected to image analysis, which resulted in angle of orientation distribution of the constituent structures (black speckle in top right corner).

(2) Secondly, analytic understanding was created by understanding, how the results that we derived for EM responses are related to existing results to be found research literature. In addition to deriving a new type of mixing formula for multiple statistically independent filler species, we showed that it reduces to Maxwell-Garnett type of classical results in the limit of vanishing microgeometry corrections.

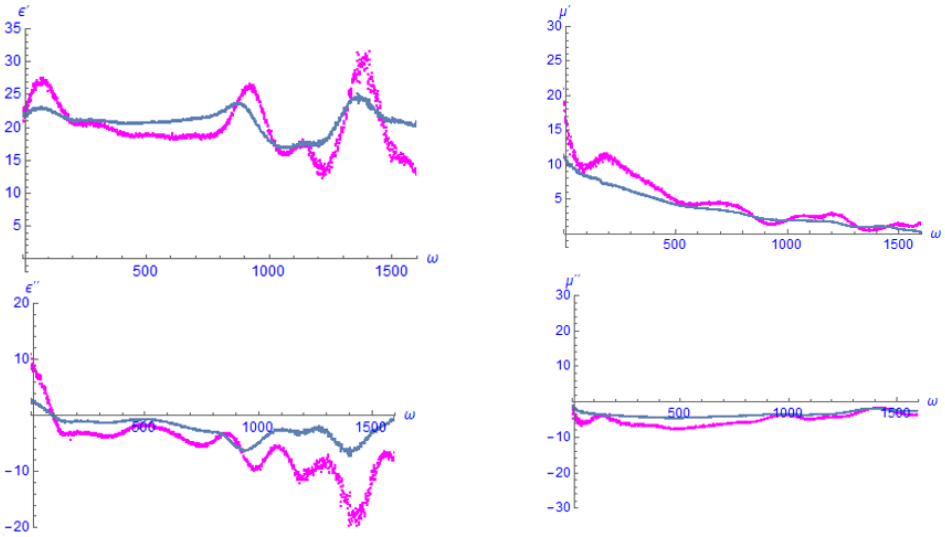

Fig.3. Inverse engineered real (top) and imaginary parts (bottom) of permittivity (left) and permeability (right) for spherical ferroelectric filler particles having volume ratios 5.5% (magenta) and 16.7% (dark blue). The frequency (x-axis) has 1600 data points in the range 0.5 GHz to 18 GHz.

As this result represents the predictive capabilities of our framework, we also utilized

the known classical mixing formulae in reverse engineering (Fig.3) the individual filler particle permeabilities and permittivities, which created the basis for the predictive model building. The accuracy of the reverse engineering results was verified by using the classical mixing formulae to predict the EM responses of e.g. a 3 species composite (2 filler species + matrix), the results agreeing within a few percent margin over wide spectral range. (3) Finally, we isolated from the surrogate level models the most crucial component to be subjected to AI techniques to speed up the computation of the numerical predictions. Over three orders of magnitude (> 1000) speed up was achieved between the most accurate type A surrogate and the type B surrogate constructed by machine learning.

The predictive surrogate framework created in this work is not totally novel, as we were able to anchor it to many existing theories. This is not surprising given the fact that we required that in certain limits it must reduce to some known theories (e.g. Maxwell-Garnett) as do many other, though not all, theories. So, there is bound to be some overlap between these types of theoretical formulations. Also, the statistical averaging techniques we utilized are not new. The positive side, of course, is that due to the overlap, we are able to utilize many known results from literature for 'free' and we can use certain limits as 'anchor' points to give more credibility for our choices. Due to the verifiable framework, it is now possible to advance further in certain respects than what has been done in the existing literature. For example, state of the art can be improved as what comes to the inclusion of statistical interaction of different particle species, higher order correlation functions, new type of filler geometries and use of anisotropies in observed distributions such as the non-monotonicity of the filler particle angles mentioned in Sect. 3. Naturally, all this leads to more complicated numerical expressions to be computed, and therefore development of further AI based surrogate models to speed up the calculation is also necessary.

To create a computable framework in a finite time frame, we left out from the current formulation certain parameter extremization steps, which can play a more pronounced role in theories containing higher order correlation functions. The inclusion of higher order corrections leads to the development of AI based surrogates different from the present work. We also used oversimplified micro-geometrical approximations for the filler particles by taking them to be spherical or ellipsoidal. This led to observations about the smallness of the novel micro-geometry related correction terms as compared to parametric uncertainties resulting from experimental measurements and other error sources. This, in turn, motivated us to consider, how the 'signal' could be amplified as compared to the noise leading to the introduction of ellipsoidal filler particles with extremely large semi-axis ratio (Fig.4). Interesting morphological changes were observed in the design parameter space for EM response functions in this anisotropic limit. Further investigation is required to determine if these types of effects do persist for realistic fillers such as carbon nanotubes while at the same time performing averaging over correct size, axis orientation and other distributions. In the current work only the centers of mass of the fillers were correctly averaged over, while the sizes and orientations of ellipsoids were assumed fixed leading to anisotropic ordering. Anisotropy in the tensorial form of the permittivities and permeabilities was also left out in this work as we have utilized trace averaging in the expressions of the EM responses (average of the diagonal elements).

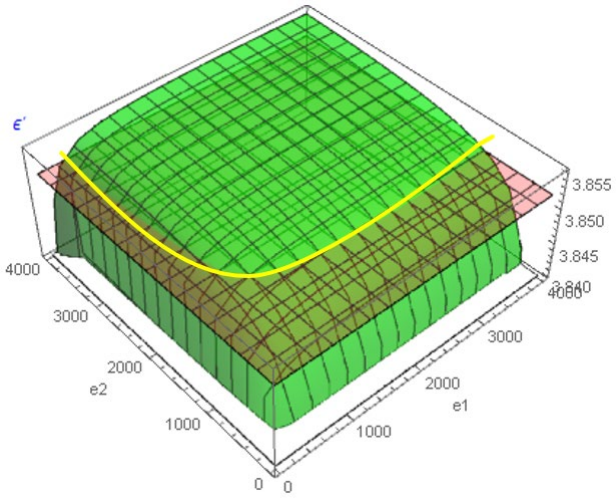

Fig.4 Portion of the design space of 3-component mixture with two filler species, whose individual permeabilities have been denoted with e1 and e2. On the z-axis is shown the predicted real part of the permeability of the mixture by the surrogate model. The pink plane indicates a hypothetical target value of the permeability. The intersection of these two 2D surfaces is indicated by the yellow line. The optimal mass solution is obtained by traversing along the yellow constraint curve and searching for a point which minimizes expression for the composite mass. With larger dimensional design parameter space, the constrained curve (surface) is more convoluted requiring the use of a fast-to-compute surrogate in the optimization process.

5. Conclusions

We have developed a computational framework for studying the effects of micro-geometry induced effects on the permeability and permittivity of multi-component mixtures in single layer systems (multi-layer optimization is enabled by single layer results). Owing to the sound theoretical anchoring we established, it should be rather straightforward to set up a numerical pipeline, which can utilize the types of truly novel extensions of our micro-geometrical correction terms introduced in Sect. 4.

To increase the degree of novelty further, we could include new types of experimentally determined micro-geometry distribution data in the process. Additionally, there are several things that could be tested: the behavior of higher order correction terms for large permittivity differences between filler particles (cf. graphite vs. Carbonyl iron) and signal-to-noise amplification with large semi-axes ratios of filler particles. Cross-correlation effects in multi-species composites could also be studied at the level of lowest order corrections. All these extensions would require the development of AI based surrogates, too. If we want to push the novelty level even higher, a separate investigation (which could be done *independently* of the EM response evaluation due to the fact that geometrical averaging can be done parallel in our formalism) could be undertaken focusing on the use of more irregularly shaped filler particles. This study could be purely numeric and aim at simply calculating the lowest (2^{nd}) order geometric correlation functions, which could be directly inputted into our analytical prediction framework.

However, before pushing the envelope too far with respect to micro-geometry aspects,

we should take the current exercise to its logical end by performing a proper optimization with all practical constraints implemented. This would mean that the optimizer would recognize relevant experimental constraints related to mixture preparation, macroscopic structure of irradiated object (layer parameters etc.) together with the mass minimization requirement. The building blocks for this type of total optimization tool already exist and owing to the present contributions we are a step closer to reaching verifiable results in the very high-dimensional design space.