Mathematical Modeling of Metamaterials

Yuri Godin, **Lead**
Stanislav Molchanov
Boris Vainberg

Department of Mathematics and Statistics,
University of North Carolina at Charlotte,
Charlotte, NC 28223

Target category: Existing and Emerging Excellence

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Executive Summary

A metamaterial is an artificially engineered material to has a property that is not found in naturally occurring materials. They are made from assemblies of multiple elements fashioned from composite materials such as metals and plastics. The materials are usually arranged in repeating patterns, at scales that are smaller than the wavelengths of the phenomena they influence. Metamaterials derive their properties not only from the properties of the base materials, but mostly from their newly designed structures. A strong interest in the subject had led to the establishment in 2007 of a special peer-reviewed scientific journal *Metamaterials* published by Elsevier in association with the Metamorphose Network of Excellence, as well as the annual International Congress on Artificial Materials for Novel Wave Phenomena – Metamaterials.

Metamaterials are categorized according to the type of wave they are intended for.

Electromagnetic metamaterials

One example of such material is a photonic crystal which is an artificial periodic dielectric or metallo-dielectric nanostructure that supports the propagation of optical waves of a certain frequency and suppresses the propagation of the others. One-dimensional photonic crystals are already in widespread use, in the form of thin-film optics, with applications from low and high reflection coatings on lenses and mirrors to color-changing paints and inks. The first commercial products involving two-dimensionally periodic photonic crystals are already available in the form of photonic-crystal fibers, which use a microscale structure to confine light with radically different characteristics compared to conventional optical fiber for applications in nonlinear devices and guiding exotic wavelengths.

Mechanical metamaterials are designed to control, direct, and manipulate sound or elastic waves in gases, liquids, and solids. With mechanical metamaterials, the direction of sound through the medium can be controlled by manipulating the acoustic refractive index. Therefore, the capabilities of traditional acoustic technologies are extended, for example, eventually being able to cloak certain objects from acoustic detection. The first successful industrial applications of acoustic metamaterials were tested for aircraft insulation.

More than a million earthquakes are recorded each year, by a worldwide system of earthquake detection stations. Computations showed that seismic waves traveling toward a building could be directed around the building, leaving the building unscathed, by using seismic metamaterials. A seismic metamaterial is a metamaterial that is designed to counteract the adverse effects of seismic waves on artificial structures, which exist on or near the surface of the earth. The very long wavelengths of earthquake waves would be shortened as they interact with the metamaterials; the waves would pass around the building to arrive in phase as the earthquake wave proceeded as if the building was not there. Current designs of seismic metamaterials utilize configurations of boreholes, trees, or proposed underground resonators to act as a large scale material.

Evidence of Strength and Excellence

Yu. Godin, S. Molchanov, and B. Vainberg have a successful experience of collaboration working together over 20 years and have five joint articles published in the world's leading journals on Applied Mathematics. In addition, S.M. and B.V. published 35 joint papers, Yu.G. and B.V. published 9 joint papers, and Yu.G. and S.M. published 3 papers jointly. The conjunction of the unique experience of each member of the group allowed them to solve several topical problems for metamaterials by combining ideas from the areas of differential equations with random coefficients, acoustic and electromagnetic waves, localization, and perturbation theory. The group has a weekly seminar on Mathematical Physics where its participants as well as graduate students report their most recent results. The close relationship between the group members developed the synergy of the team to solve the longstanding problems in the composites and metamaterials. The results were also reported on national and international conferences including

- International Congress on Industrial and Applied Mathematics, Valencia, Spain
- SIAM Conference on Mathematical Aspects of Materials Science
- The 10th European Solid Mechanics Conference, Bologna, Italy
- International Conference on Mathematical and Numerical Aspects of Waves Propagation

and more. More specifically,

Prof. S. Molchanov is a fellow of the American Mathematical Society. He is an author of four monographs and more than 250 papers in the leading mathematical journals and a world renown expert in mathematical physics, random processes and their applications, quantum graphs, homogenization, localization, intermittency, fractals, population dynamics, and more. Prof. Molchanov is a member of the Editorial Boards of the journals *Random Operators and Stochastic Equations*, *Journal of Spectral Theory*, and *Mathematical and Theoretical Physics.* In the last five years alone, he has been supported by two grants from the NSF, one grant from the Russian Science Foundation and a research grant from Bielefeld University (Germany). He has supervised 17 Ph.D. students.

Prof. B. Vainberg is a world leading expert in partial differential equations, mathematical physics, scattering theory, asymptotic methods, inverse problems, free surface hydrodynamics, acoustic and electromagnetic waves, population dynamics and more. He is an author of three monographs, a chapter in another monograph and about 180 papers. Prof. Vainberg is a member of the Editorial Board of the journal *Applicable Analysis.* In the last five years alone, he has been supported by two grants from the NSF and a grant from the Simons Foundation. He has supervised four Ph.D. students.

Dr. Yu. Godin is a specialist in applied mathematics, propagation of waves in periodic and random media (photonic crystals), overall properties of composites, numerical calculations. He was an organizer of two SIAM minisymposia on Mathematical Aspects of Materials. He served as a member of Ph.D. committees for many doctoral students.

Here are some examples of the research impact of the group.

- It has been believed among the physicists that a drastic slowdown of the acoustic wave velocity in liquids containing even a tiny concentration of air bubbles can be explained by so-called Minnaert resonance, that is when the air bubbles resonate at the wave frequency that impedes wave propagation. In our just accepted paper, we show that this assumption is actually wrong and provide a rigorous explanation of this phenomenon. The new approach suggested in our paper makes it possible to design novel composite materials that dramatically reduce the speed of wave propagation.

- With the widespread use of photonic crystals in applications, it soon became clear that manufactured photonic devices do not demonstrate theoretically predicted properties if the frequency of the propagated wave is near the band-edge of the transmission spectrum. We started investigating this effect and found the crystal fabrication requires much higher accuracy when the frequency of wave propagation is close to the bandedge. Moreover, in our paper, we provided a rigorous description of the Lyapunov exponent of the waveguide transmission as a function of the magnitude of the disorder and the location of the wave frequency in the band.

- There is immense current interest in wave phenomena in artificial periodic media. The varied and sometimes unexpected, wave propagation properties of composites have motivated a number of remarkable new applications, including, photonic crystals, as well as the rapidly developing area of metamaterials. Thus, there is considerable interest in modeling wave propagation through media with regularly spaced defects or inhomogeneities. Direct numerical simulation using finite elements is popular but can become intensive for large-scale media with many small inclusions. Complementary to this literature is that of homogenization, which involves taking a medium with rapidly oscillatory material properties on a fine microscale and averaging these out, in some fashion, to obtain an equivalent homogeneous material with effective material parameters. Propagating waves in such medium exist only at a certain relation between temporal and spatial frequency, called the dispersion relation. Finding this relation is an arduous problem, especially in two-dimensions, and even more so in a three-dimensional case, but this knowledge is crucial for understanding wave propagation. Our recent publication suggests a novel approach that allows deriving dispersion relations for both two and three-dimensional periodic metamaterials.

Numerical evaluation of properties of metamaterials and subsequent graphical illustration requires modern computational resources and software. Summer support for faculty and students may significantly advance the success of the project.

Alignment with Regional and National Priorities

The importance of advanced materials with novel properties not found in naturally occurring materials – metamaterials – has already been realized by all scientific and engineering entities. Here are some examples of the involvement of state and federal agencies in the support of the development of metamaterials.

- National Science Foundation (NSF) has several divisions supporting metamaterial research. They include the Division of Materials Research (DMR), the Directorates for Mathematical and Physical Sciences (MPS), Engineering (ENG), and Computer & Information Science & Engineering (CISE), Designing Materials to Revolutionize and Engineer our Future (DMREF). Over the recent years, NSF has awarded over 140 grants to research related to metamaterials.
- Several divisions of the Air Force Research Laboratory (AFOSR) are interested in research and technologies involving metamaterials and their applications. They include the divisions of Aerospace Components & Subsystems Technology (AFRL/RYD), Multispectral Sensing & Detection Division (AFRL/RYM), the division of Physical Sciences (AFOSR).
- Society for Industrial and Applied Mathematics (SIAM) – the world's largest professional association devoted to applied mathematics – organizes special sections during its annual meetings dedicated to modeling, analysis, and design of metamaterials. One of its activity groups – Mathematical Aspects of Materials Science – organizes every other year conferences and minisymposia where mathematical problems associated with metamaterials are discussed.
- The Virtual Institute for Artificial Electromagnetic Materials and Metamaterials "Metamorphose VI AISBL" is an international association to promote artificial electromagnetic materials and metamaterials. It organizes scientific conferences, supports specialized journals, creates and manages research programs, provides training programs (including PhD and training programs for industrial partners); and technology transfer to European Industry. One of the main topics of the forthcoming Fifteenth International Congress on Artificial Materials for Novel Wave Phenomena – Metamaterials 2021 which is expected to be held on August 2 - 7, 2021 in New York, USA, will be
  - Analytical and numerical modeling of metamaterials and metasurfaces
  - Homogenization and effective medium models
- One of the Industry-University Cooperative Research Centers (IUCRC) affiliated with the National Science Foundation is located at the University of North Carolina, Charlotte. The Center for Metamaterials (CfM) designs, fabricates and tests a wide range of metamaterials. Its mission is to advance fundamental and applied metamaterials research, development, and technology transfer through strong collaborations between industry and universities. There is strong industry interest in metamaterials, as they are being used to develop new or higher-performing optical, electronic, and acoustic devices.

Supporting Documents

Names	Titles	Expertise
Yuri Godin	Associate Professor	Applied mathematics, propagation of waves in periodic and random media (photonic crystals), overall properties of composites, numerical calculations
Stanislav Molchanov	Full Professor	Mathematical physics, partial differential equations, random processes, and their applications: scattering theory, oceanography, quantum graphs, homogenization, localization, intermittency, fractals, population dynamics, etc.
Boris Vainberg	Full Professor	Mathematical physics, partial differential equations, scattering theory, asymptotic methods, inverse problems, free surface hydrodynamics, acoustic and electromagnetic waves, population dynamics and more