materials proceedings

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Proceeding Paper

Fine-Tuning Collective Atomic Vibrations in Low-Dimensional Nanocarbon Multilayer Transition Interfaces for 3D Printed Extreme Lattice Metamaterials Performance Improvement †

Alexander Lukin

Western-Caucasus Research Center, Tuapse 352808, Russia; lukin@wcrc.ru; Tel.: +7-918-3080-916

† Presented at the 4th International Online Conference on Nanomaterials, 5–19 May 2023; Available online: https://iocn2023.sciforum.net.

Abstract: We have developed a game-changing approach for additively manufactured extreme lattice metamaterials predictive performance improvement and unlocking the new functionalities via fine-tuning atomic vibrational inter-layer interactions within the transition domains of multilayer nano-components. The developed approach is based on the recently discovered fundamental phenomenon of collective atomic vibrations, manifested within transition domains of multilayer nanostructures. For predictive excitation and adjustment of this phenomenon, we propose incorporation of the low-dimensional nanocarbon-based multilayer interfaces into the transition domains of nanocomponents via a multistage technological chain. In particular, this chain includes combination of a set of techniques: conversion of all components into the nanoscale, the plasma-driven functionalization and assembling with multilayer nano-enhanced interfaces, the energy-driven initiation of the allotropic phase transformations, the surface acoustic waves-assisted micro/nano- manipulation during the ion-assisted pulse-plasma functionalizing, the heteroatom doping, initiating directed self-assembly through application external high-frequency electromagnetic fields, the resonant acoustic mixing of all nanocomponents, growing the high-end extreme lattice metamaterials elements by high-precision multi-material additive manufacturing as well as using the data-driven digital twins-based nanoscale manufacturing approach.

Keywords: extreme lattice metamaterials; low-dimensional sp-hybridized carbon nanostructures; 2D-ordered linear-chain carbon; multilayer nano-enhanced interfaces; collective atomic vibrations; heteroatom doping; multi-material additive manufacturing; data-driven nanoscale manufacturing approach; cyber-physical systems

Citation: Lukin, A. Fine-Tuning Collective Atomic Vibrations in Low-Dimensional Nanocarbon Multilayer Transition Interfaces for 3D Printed Extreme Lattice Metamaterials Performance Improvement. *Mater. Proc.* **2023**, *5*, x. https://doi.org/10.3390/xxxxx

Published: 5 May 2023

1. Introduction

The development of advanced lightweight materials with precisely selected combinations of the required nano-topological, mechanical, thermal and other physical and chemical properties is the “Holy Grail” of nano-materials science. The structure-property relationship is the most important paradigm in materials science. While most modern materials demonstrate a set of unique properties due to their material composition and corresponding technological processing, the unique topological and physicochemical properties of nanostructured metamaterials arise not from the properties of the raw materials used, but due to the specific features of the spatial distribution of components, for instance, in the form of periodic structures, their mutual orientation and unusual geometric characteristics.

The extreme lattice metamaterials (ELM) with a set of unprecedented topological and physicochemical properties, in fact, represent a new type of matter that does not usually exist in nature, and can be considered as promising nanoscale building blocks.

Multi-functional lattice structures utilizing metamaterials have the potential to radically change the future of products that we use in our daily lives and the way in which industries like aerospace and the medical field operate, [1].

In the context of additive manufacturing, lattice structures open up unique design possibilities as 3D printing technologies uncover possibilities for creating shapes and parts that were previously "unmanufacturable".

On Figure 1 lists some characteristics of extreme lattice metamaterials that are of particular interest to a wide range of research and engineering applications.

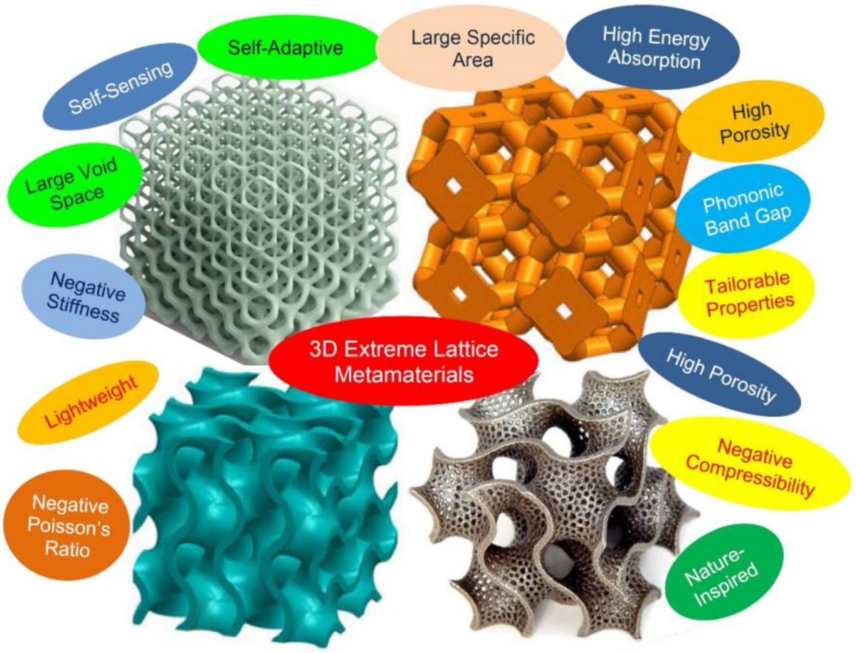

Figure 1. Overview of 3D extreme lattice metamaterials: structure-property relationship.

The further evolution of these metamaterials is "field-responsive mechanical metamaterials", which are capable of almost instantly responding and stiffening 3D printed structures when exposed to an external magnetic field. The use of 3D printing technology allows the growed objects to feel the external forces applied to them for use in advanced interactive applications.

Currently available high-precision multi-material additive manufacturing techniques uncover practically limitless possibilities for the rational design of unique extreme lattice metamaterials, not only with complex topologies, as well as with arbitrary distributions of multiple materials within the selected topologies, resulting in unique sets of combinations of topological and physicochemical properties. In particular, additive manufacturing allows combining multiple materials within a single topological component.

2. Fine-Tuning Vibrational Interactions

The origin of physicochemical properties, nano-topology and functionality for nanomaterials is at atomic scale. Important vibrational, mechanical, thermal, electronic and transport characteristics of nanomaterials are controlled by phonons: by the propagating atomic vibrational waves.

Recent fundamental discovery, based on study of atomic-resolution imaging, confirmed excitation of collective atomic vibrations in nanoscale systems, called phonon waves, [2]. In particular, these vibrations or "phonon waves" determine the processes of transfer of electric charges and heat in nanomaterials. In accordance with this discovery, phonons can generate a wave that has capability transfer across all subsequent materials, also known as a coherent effect. Phonons play a decisive role in formation of the physical properties of nanomaterials. This explains why nanoscale interfaces are capable of demonstrating the unique properties that are different from the neighboring nanomaterials.

Within the multilayer nanomaterials, the phonon waves, manifested in transition domains of multilayer nanostructures, are capable of inducing collective vibrational interaction with related materials at the nanoscale.

In other words, desired nanomaterial properties can be achieved by changing how different layers or components couple to each other, by changing the number of interacting layers as well as their thicknesses. For nanolayers smaller than 10–20 nm, vibrations of the most external atomic layers are relatively large and hence play a significant role in formation of its properties.

The ability to manipulate by collective atomic vibrations uncover access to predictive programming the physicochemical priorities of the lattice metamaterials.

Based on fundamental phenomenon of collective atomic vibrations, manifested within transition domains of multilayer nanostructures, we have developed a game-changing approach for additively manufactured ELM predictive performance improvement and unlocking the new functionalities via fine-tuning atomic vibrational inter-layer interactions within the transition domains of multilayer nanocomponents.

For predictive excitation and adjustment of this phenomenon, we propose incorporation of the low-dimensional nanocarbon-based multilayer interfaces into the transition domains of nanocomponents via a multistage technological chain. In particular, this chain includes combination of a set of techniques: conversion of all components into the nanoscale, the plasma-driven functionalization and assembling with multilayer nano-enhanced interfaces, the energy-driven initiation of the allotropic phase transformations, the surface acoustic waves-assisted micro/nano- manipulation during the ion-assisted pulse-plasma functionalizing, the heteroatom doping, initiating directed self-assembly through application external high-frequency electro-magnetic fields, the resonant acoustic mixing of all nanocomponents, growing the high-end ELM elements by high-precision multi-material additive manufacturing as well as using the data-driven digital twins-based nanoscale manufacturing approach. The proposed technological chain is schematically shown in Figure 2.

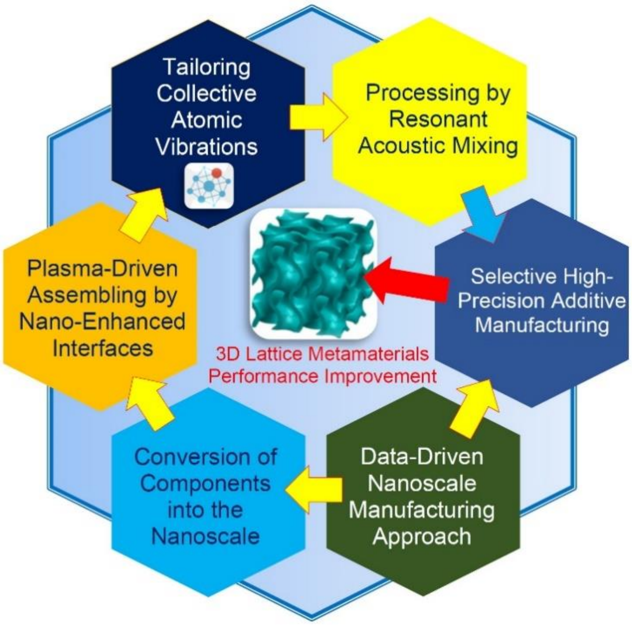

Figure 2. Schematic representation of the multistage technological chain.

These multilayer nano-enhanced interfaces also can serve as nanocarriers for heteroatom doping, as a sensitive nano-links for external electromagnetic fields as well as empower a material with the ability to "sense" its structural health.

As a promising multilayer nano-enhanced interfaces, we propose to use the low-dimensional nanocarbon allotropes with a set of unique properties.

The "Holy Grail" of low-dimensional carbon allotropes, the carbyne, represents a one-dimensional chain of carbon atoms. The growth of the macroscopic crystals of carbyne is inhibited by the instability and high reactivity of this allotropic form of carbon, which hinders the possibility of its practical use.

Relatively recently, an original route to compensate for the high reactivity of the carbon chains was found, [3]. In particular, a technique to encapsulate the oriented linear chains of carbon atoms—the monatomic carbon filaments into the matrix of amorphous carbon during the ion-assisted pulse-plasma deposition, were developed.

In accordance with the topology of the grown nano-matrix it was named as an 2D-ordered linear-chain carbon. Due to the exceptional set of properties this new nanomaterial behaves can serve as an excellent multilayer nano-enhanced interface. The spatial configuration of a 2D-ordered linear-chain carbon nano-matrix represents a two-dimensionally distributed hexagonal array of parallel one-dimensional carbon chains interconnected by the van der Waals forces and oriented perpendicular to the substrate surface, (Figure 3).

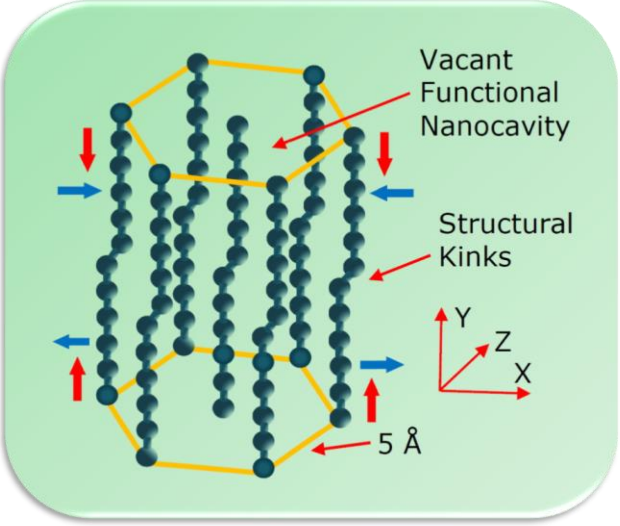

Figure 3. Schematic representation of a fragment of a 2D-ordered linear-chain carbon structure.

The distance between carbon chains is estimated as 5 angstroms. 2D-ordered linear-chain carbon nano-matrix represents a multicavity structure containing vacant functional nanocavities available for incorporating atom clusters of various chemical elements.

The 2D-ordered linear-chain carbon-based multilayer nano-enhanced interfaces has a set of specific properties that can be used for manipulating phonon waves excitation and propagation.

For ELM predictive performance improvement and unlocking the new functionalities, we propose using combination of a set of techniques for fine-tuning collective atomic vibrations and vibrational inter-layer interactions within the transition domains of multilayer interfaces.

The combination of multiple carbon nanostructured materials with various hybridizations within a single substance can uncover new unique properties.

For manipulating phonon waves propagation through predictive combining of multiple differently hybridized nanocarbons within a single substance we propose to use the energy-driven initiation of the allotropic phase transformations within multilayer nano-enhanced interfaces by concurrent electron beam and ion irradiation. The mechanism of this effect is associated with competition between formation and breaking of carbon bonds with different types of hybridization.

With taking into account that the 2D-ordered linear-chain carbon-based multilayer nano-matrix are acoustically sensitive nanomaterial, we propose assisting the nano-matrix growth, combined with heteroatom doping, by the Rayleigh-type surface acoustic waves, accompanied by patterning phenomena, leads to significant modification in the nanoarchitectures and vibrational characteristics, [4]. Application of combinations of various acoustic exciting frequencies and waveforms, generated in the nano-matrix growth zone, excites specific unified templates that provided spatial markings for the multilayer nano-matrix growing, as well as provided programming the required nanoarchitecture of the grown nanostructures.

The vibrational interactions and energy exchange within the growing nano-matrix can be enhanced by using external electromagnetic fields. Relatively recent experimental research of Rice University discovered a new phenomenon that uncovered a pathway for the direct self-assembly of the low-dimensional nanocarbon allotropes, [5]. In accordance with this discovery, nanocarbon allotropes, as well as other kinds of nanomaterials, can self-assemble at relatively large distances depending on the energy of the applied high-frequency electromagnetic emission. For instance, the carbon nano-tubes under influence of a Teslaphoresis force field, show polarization and self-assembly into the relatively long chains at macro-level as well as acquire the properties of conductors of electric current.

With a small chemical doping, the 2D-ordered linear-chain carbon-based nano-matrix can be transformed into a controllable piezoelectric material. Assembling the 2D-ordered linear-chain carbon-based nano-matrix by the piezoelectric nanomaterials clusters, for instance, by lithium atoms or zinc oxide (ZnO) nanoparticles, can transform them into the piezoelectric nanogenerators that can be used to control the electric charge distribution within the multilayer nano-matrix growing zone.

3. Data-Driven Nanoscale Manufacturing Approach

The important feature of the multilayer nano-enhanced interfaces is the ability to fine-tune their nanoarchitectures and physicochemical properties. However, without using the deep materials informatics approach, such tuning through trial and error is extremely difficult. For predictive unlocking of unique structural and physicochemical properties of the 2D-ordered linear-chain carbon-based multilayer nano-enhanced interfaces we propose the data-driven nanoscale manufacturing approach, based on data and deep materials informatics, [6]. The proposed data-driven nanoscale manufacturing approach establishes linkages between key modes and technological parameters of the ion-assisted pulse-plasma growing of the 2D-ordered linear-chain carbon-based multilayer nano-enhanced interfaces and target combinations of their nanoarchitecture and physicochemical properties through using a set of multifactorial computational models, developed with using extensive experimental data for a specific set of key descriptors.

The design strategy involves identification of key descriptors for a specific experimental system and development of the multifactorial computational models corresponding to these descriptors. Identification and characterization of key descriptors is carried out on the basis of extensive experimental data on the influence of various factors on the process of growing 2D-ordered linear-chain carbon-based multilayer nano-enhanced interfaces. The use of formalized universal linkages opens up new opportunities for forecasting modification of target nanoarchitectures and physicochemical parameters for various combinations of the ion-assisted pulse-plasma deposition and, conversely, to predict a set of required technological modes based on a combination of sets of required structural and physicochemical parameters of the nano-enhanced interfaces.

Integration of the Industry 4.0 & 5.0 interfaces into the online interface of the big data mining analytical platforms unlocked new possibilities for express development of the unique ELM with programmable properties for various applications.

4. Conclusions

Establishing and programming interactions between collective atomic vibrations, nanoarchitecture and functionality along with deep materials informatics is a key feature for discovery of new extreme lattice metamaterials with a set of unique properties.

The proposed approach uncovered the new possibility for the transition of the lattice metamaterials from the category of ordinary materials to smart, adaptive and versatile materials that can solve complicated tasks in a number of high-end systems and applications.

Funding: This research work is jointly supported and funded by the Scientific and Technological Research Council of Turkey (TÜBİTAK) and the Russian Foundation for Basic Research (RFBR) according to the research project No. 20-58-46014. The APC was funded by the Russian Foundation for Basic Research.

Institutional Review Board Statement: Not applicable.

Informed Consent Statement: Not applicable.

Data Availability Statement: Not applicable.

Acknowledgments: The publication cost of this paper was covered by funds from the Russian Foundation for Basic Research (RFBR) according to the research project No. 20-58-46014.

Conflicts of Interest: The authors declare no conflict of interest.

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