



Abstract

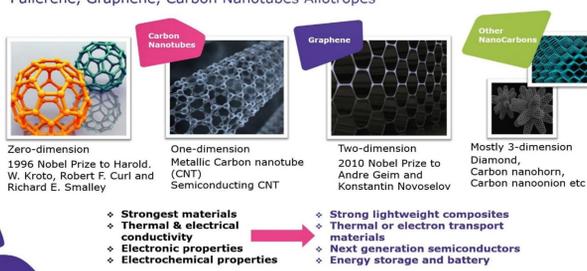
For a number of space applications require power sources that deliver high power in reliable and sustained ways over long periods of time. The direct conversion of heat into electricity without any intermediate steps or moving parts remains one of the most promising but challenging methods of energy generation. The objective of the presented research is to solving a scientific problem - increasing the energy efficiency of the method of thermionic conversion of thermal energy into electrical energy through the creation and use of a new type of emission nanomaterials - multilayer carbyne-enriched 3D-shaped nano-interfaces and fine-tuning of their topological, physicochemical and functional characteristics.

Based on recently discovered fundamental phenomenon of collective atomic vibrations, manifested within transition domains of multilayer nanostructures, called phonon waves, we developed the new concept for improving the efficiency of thermionic energy converters by predictive functionality unlocking of the 2D-ordered linear-chain carbon-based multilayer emitters through excitation and fine-tuning the collective atomic vibrations and nanoarchitecture. For predictive excitation and adjustment, the interface effects, phonon waves propagation, energy exchange and synergistic effects provided by the multilayer nano-enhanced interfaces we propose using a combination of a set of techniques. The developed approach opens up the possibility of creating devices for thermionic energy conversion of a new type, the energy efficiency of which can significantly (by orders of magnitude) exceed the efficiency of existing plasma thermionic converters. Electricity generating sources based on a thermionic conversion are considered as basic options for the development of Lunar and Martian research missions.

Background

Despite having a huge potential as an efficient direct energy conversion device, the progress in vacuum-based thermionic energy converters development has always been hindered by the space charge effect and unavailability of materials with low work function. The creation of low work function materials is critical for power conversion and electron emission applications. The work function is, in fact, a measure of how intensely a particular material is able to hold its electrons. Emission electrons carry away a significant amount of thermal energy from the emitter, but only a part of it can be directly converted into electrical energy. Over the past few decades, carbon-based nanomaterials and, specifically, low-dimensional nanocarbon allotropes have revolutionized the field of materials science.

Carbon Nanomaterials Family



The "holy grail" of low-dimensional carbon allotropes, carbyne, represents a one-dimensional chain of carbon atoms.

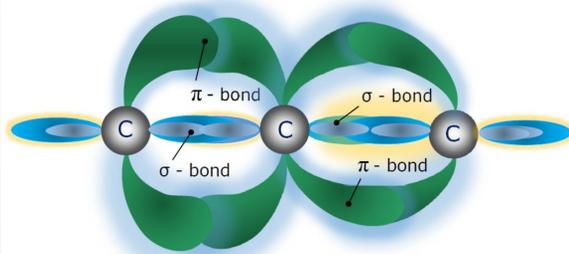


Fig. 1. The electronic structure of a fragment of a linear-chain carbon molecule section.

The advantage of carbyne for field emission applications is the high mobility of charge carriers and the strong anisotropy of the electrical resistance along the chains of carbon atoms and between the chains. Carbyne carbon chains are efficient electron emitters, and the crystalline phase has a low electron work function. The anomalously low work function of carbyne microcrystals can be explained by the superposition of the internal micro-fields of the carbon chains that make up the crystals. The growth of the macroscopic crystals of carbyne is inhibited by the instability and high reactivity of this allotropic form of carbon.

Relatively recently, an original route to compensate for the high reactivity of the carbon chains was found. In particular, a technique to encapsulate the oriented linear chains of carbon atoms into the matrix of amorphous carbon during the ion-assisted pulse-plasma deposition, was developed. In accordance with the features of the obtained spatial topology, the grown nano-matrix was named as an 2D-ordered linear-chain carbon. This new nanomaterial behaves as an excellent electron-field emitter owing to its exceptional properties and offers several benefits compared to traditional cathodes.

New Approaches and Methods

Since the origin of the physicochemical properties and functional characteristics of nanomaterials is at the atomic scale, the predictive manipulation of collective atomic vibrations within nanolayers is the key to designing multilayer emission nano-systems with unique properties. Based on recently discovered fundamental phenomenon of collective atomic vibrations, manifested within transition domains of multilayer nanostructures, called phonon waves, we developed the new concept for improving the efficiency of thermionic energy converters by predictive functionality unlocking of the 2D-ordered linear-chain carbon-based multilayer emitters through excitation and fine-tuning the collective atomic vibrations and nanoarchitecture.

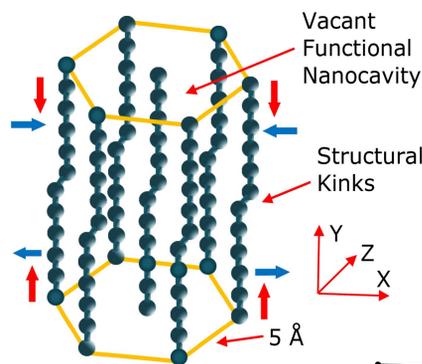


Fig. 2. Geometric characteristics of the two-dimensionally ordered linear-chain carbon nano-matrix.

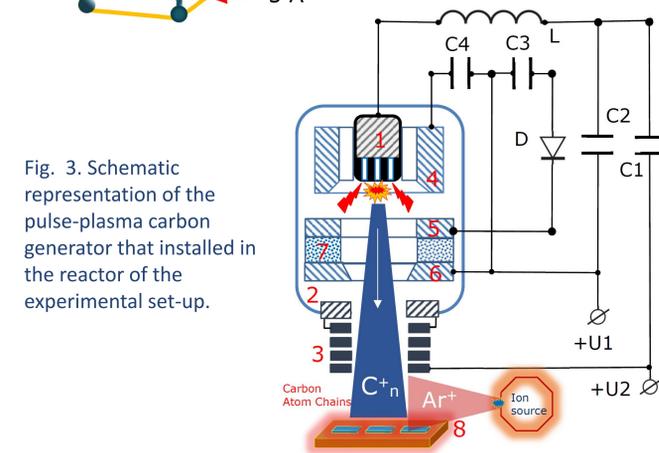


Fig. 3. Schematic representation of the pulse-plasma carbon generator that installed in the reactor of the experimental set-up.

The performance of devices for energy conversion is intimately linked to the ability of materials to form complex heterogeneous 3D-shaped interfaces. Planar nano-interfaces are considered as a "basis" that can be modified or upgraded to 3D-shaped nano-interfaces. Using the surface acoustic waves (SAW) allows to generate 3D-shaped nano-interfaces with complex geometry. For fine-tuning and programming of the nano-interface-based and synergistic effects (self-synchronization of collective atomic vibrations, phonon waves propagation, energy exchange) within the multilayer 3D-shaped nano-enhanced interfaces we developed a set of tool-kits: - initiation and programming of phase transformations in grown nano-layers by combining ion and electron irradiation with different doses; - heteroatomic doping with clusters of atoms of various chemical elements; - stimulation of the growing zone by surface-acoustic waves; - stimulation of the growing zone by remote exposure to high-frequency electromagnetic fields; - initiation in the zone of growing the phenomenon of "explosive" directional self-assembly of carbyne-enriched nanostructures; - the use of data-driven digital twins-based nanoscale manufacturing approach.

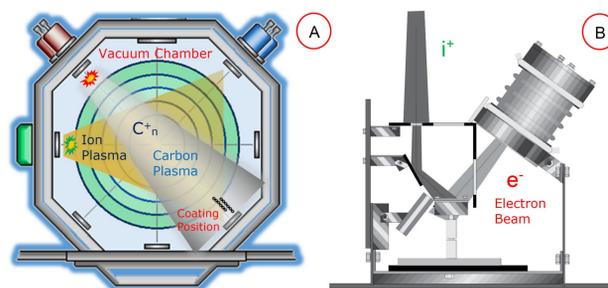


Fig. 4. Schemes of the experimental set-ups for concurrent electron beam and ion-irradiation of the 2D-ordered linear-chain carbon-based multilayer nano-enhanced interfaces: (A) - pulse-plasma deposition reactor; (B) - combination of the ion sputtering of a graphite target simultaneously with electron beam irradiation using an electron gun.

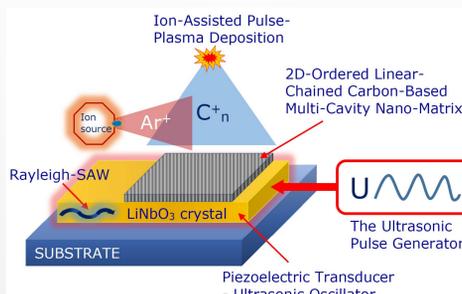


Fig. 5. Schematic representation of application of the inverse piezoelectric effect during the ion-assisted carbon pulse-plasma deposition.

Results

The scientific novelty of the research lies in the development of a new strategy for growing samples of emission nanomaterials of a new type - data-driven information technology tools and the development of advanced technological methods and methods for growing new types of multilayer emission nanomaterials with a programmable complex of unique structural and physicochemical properties that will become the basis to create promising systems for direct energy conversion.

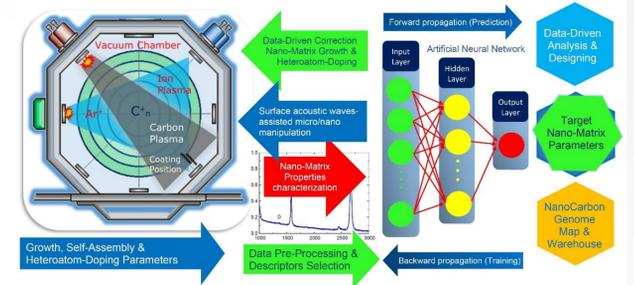


Fig. 6. Machine learning-based fine-tuning of the 3D-shaped nano-interfaces with complex geometry: a scheme of tracking and tailoring the key descriptors and linkages for incorporating into the data-driven carbon nanomaterials genome approach.

A set of interacting 3D-shaped nano-interfaces can be considered as nanodevices. The schematic representation of interactions of the effects and phenomena used for fine-tuning the artificially structured multi-layered transition nano-enhanced interfaces properties is presented in Figure 7.

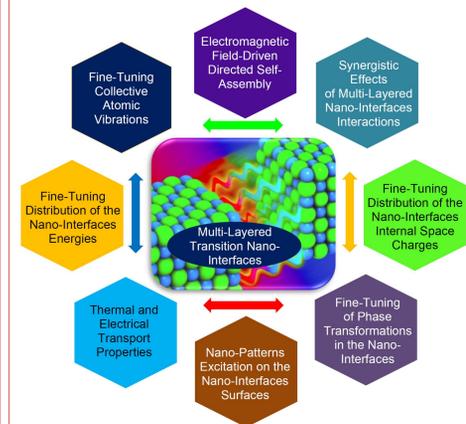


Fig. 7. Fine-tuning the artificially structured multi-layered transition 3D-shaped nano-enhanced interfaces properties and their synergistic effects.

Conclusion

We developed the new concept for improving the efficiency of thermionic energy converters by predictive unlocking the multilayer low-dimensional nano-carbon allotropes-based emitters functionality through excitation and fine-tuning the collective atomic vibrations, functionalities and nanoarchitecture. In particular, we propose using 2D-ordered linear-chain carbon-based multilayered nano-enhanced interfaces as well as their synergistic effects.

For predictive excitation and adjustment of the nano-interface-based and synergistic effects such as self-synchronization of collective atomic vibrations, phonon waves propagation and energy exchange within the multilayer 3D-shaped nano-enhanced interfaces we developed a set of tool-kits. In particular, these tool-kits include combination of a set of techniques:

- the energy-driven initiation of the allotropic phase transformations at concurrent electron beam and ion irradiation required for manipulating phonon waves propagation;
- the surface acoustic waves-assisted micro/nano-manipulation during the ion-assisted pulse-plasma growing combined with heteroatom doping;
- initiating directed self-assembly through application external high-frequency electromagnetic fields;
- using the data-driven digital twins-based nanoscale manufacturing approach.

The developed approach opens up the possibility of creating the thermionic energy conversion systems of a new type, the energy efficiency of which can significantly (by orders of magnitude) exceed the efficiency of existing systems.

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