Concept Paper

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New Technological Approach for Improving the Thermionic Energy Conversion Efficiency for Space-Power Applications and Deep Space Exploration †

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Abstract: Power sources that can consistently deliver high levels of energy over extended periods are crucial for various space applications. Among the many methods of energy generation, direct heat-to-electricity conversion without intermediate steps or moving components shows particular promise but also presents significant challenges. The aim of this research is to address these challenges by enhancing the energy efficiency of thermionic conversion, which transforms thermal energy into electrical energy, through the development and utilization of a novel class of emission nanomaterials known as multilayer carbyne-enriched 3D-shaped nano-interfaces. By manipulating the topological, physicochemical, and functional characteristics of these interfaces, we seek to optimize their thermionic conversion capabilities. Building on the recent discovery of collective atomic vibrations called phonon waves within transition domains of multilayer nanostructures, we have devised a new approach to enhance the efficiency of thermionic energy converters. This involves unlocking the predictive functionality of 2D-ordered linear-chain carbon-based multilayer emitters through the excitation and fine-tuning of collective atomic vibrations and nanoarchitecture. To achieve this, we propose employing a combination of techniques that leverage interface effects, enable phonon wave propagation, facilitate energy exchange, and capitalize on synergistic effects offered by the multilayer nano-enhanced interfaces. The resulting devices for thermionic energy conversion have the potential to significantly surpass the efficiency of existing plasma thermionic converters by several orders of magnitude. Moreover, these electricity-generating sources based on thermionic conversion represent fundamental options for the advancement of Lunar and Martian research missions, opening up possibilities for sustainable energy production in extraterrestrial environments.

Keywords: thermionic energy conversion; carbyne; 2D-ordered linear-chain carbon; multilayer carbyne-enriched 3D-shaped nano-interfaces; phonon waves; collective atomic vibrations; synergistic effects; material genome technology; data-driven carbon nanomaterials genome approach; machine learning-powered inverse design; Lunar & Martian research missions

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Introduction

Converting heat into electrical energy, without the requirement of intermediary mechanisms or components, is a greatly promising yet arduous method within the realm of energy generation, [1, 2]. The development of vacuum-based thermionic energy converters as efficient direct energy conversion devices has always faced challenges due to the space charge effect and the lack of materials with low work function. Low work function materials are crucial for power conversion and electron emission applications, as they determine how strongly a material can hold its electrons. While emission electrons carry away significant thermal energy from the emitter, only a portion of it can be directly converted into electrical energy. In recent decades, carbon-based nanomaterials, especially low-dimensional nanocarbon allotropes, have revolutionized the field of materials science, [3]. Among the low-dimensional carbon allotropes, carbyne, which consists of one-dimensional carbon atom chains, is considered the "holy grail." Two different structures of carbyne chains can be identified: the α-phase, referred to as polyyne [chemical structure (–C≡C)n], which consists of alternating single and triple bonds, and the β-phase, known as cumulene [chemical structure (=C=C)n], comprising solely double bonds. Carbyne offers several advantages for field emission applications, including high charge carrier mobility and strong anisotropy of electrical resistance along and between the carbon chains, [4]. Crystalline carbyne microcrystals exhibit efficient electron emission and possess a low electron work function. The anomalously low work function of carbyne microcrystals can be attributed to the superposition of internal micro-fields within the carbon chains comprising the crystals. However, the growth of macroscopic carbyne crystals is hindered by the inherent instability and high reactivity of this carbon allotrope. Recently, a promising approach to overcome the reactivity limitations of carbyne chains has been discovered, [5]. Specifically, a technique has been developed to encapsulate oriented linear chains of carbon atoms within an amorphous carbon matrix using ion-assisted pulse-plasma deposition. This growth process results in a new nanomaterial known as 2D-ordered linear-chain carbon, which exhibits exceptional electron-field emission properties, [5]. Compared to traditional cathodes, this nanomaterial offers numerous advantages and holds great promise for various applications.

Generating Phonon Waves through Nano-Enhanced Interfaces in Multilayered Thin Films

In recent years, there has been an increasing emphasis on the study of nanoscale objects, which have emerged as a unique form of matter with distinct structural, physicochemical, and functional properties. These remarkable characteristics have paved the way for numerous promising applications in various fields. Exciting progress in scanning transmission electron microscopy has brought forth new opportunities to observe and analyze the distinct phonon modes and specific vibrations exhibited by impurities and dopants at the nanoscale. These advancements offer novel pathways for detailed imaging and comprehensive analysis of these phenomena. The utilization of vibrational spectroscopy techniques at the nanoscale allows for the visualization of individual phonon modes and precise mapping of low-energy phonon and plasmon excitations. This groundbreaking approach provides a fresh perspective on the complex interactions between plasmons and molecular vibrations. Furthermore, it offers valuable insights into phenomena associated with thermal and electrical transfer at interfaces, [6, 7]. Recent advancements in atomic-resolution imaging have resulted in a significant breakthrough, confirming the presence of collective atomic vibrations termed "phonon waves" in multilayer nanoscale thin film systems, [8]. This newfound understanding greatly enhances our knowledge of the behavior and dynamics of these vibrational phenomena. Specifically, the existence of "phonon waves" plays a critical role in governing the transportation of electric charges and heat within nanomaterials.

New Approaches and Methods

The manipulation of collective atomic vibrations within nanolayers is crucial for designing multilayer emission nano-systems with unique properties, as the origin of the physicochemical properties and functional characteristics of nanomaterials lies at the atomic scale. Our research has led to the discovery of a fundamental phenomenon called phonon waves, which manifest within transition domains of multilayer nanostructures. Expanding on this discovery, we have developed an innovative concept to enhance the efficiency of thermionic energy converters. Our concept focuses on unlocking the predictive functionality of 2D-ordered linear-chain carbon-based multilayer emitters by exciting and finely tuning collective atomic vibrations and nanoarchitecture.

The performance of energy conversion devices relies on the materials' ability to form complex heterogeneous 3D-shaped interfaces. While planar nano-interfaces serve as a foundation, they can be upgraded or modified into 3D-shaped nano-interfaces. To accomplish this, we harness the power of surface acoustic waves (SAW) to generate 3D-shaped nano-interfaces with intricate geometries. Furthermore, we have developed a toolkit to precisely tune and program the nano-interface-based and synergistic effects within the multilayer 3D-shaped nano-enhanced interfaces. This toolkit includes the following methods and techniques:

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- Combining ion and electron irradiation with various doses to initiate and program phase transformations in grown nano-layers;
- Heteroatomic doping using clusters of atoms from different chemical elements;
- Stimulating the growing zone using surface-acoustic waves;
- Stimulating the growing zone through remote exposure to high-frequency electromagnetic fields;
- Triggering the phenomenon of "explosive" directional self-assembly of carbyne-enriched nanostructures in the growing zone;
- Utilizing a data-driven carbon nanomaterials genome approach to guide the process.

Results

The research introduces a groundbreaking approach to cultivating emission nanomaterials by utilizing data-driven information technology tools. This strategy also involves the advancement of technological methods for growing new types of multilayer emission nanomaterials with specific structural and physicochemical properties. These innovative materials will serve as the foundation for creating cutting-edge systems capable of direct energy conversion. The diagram in **Figure 1** illustrates the interconnected 3D-shaped nano-interfaces functioning as nanodevices.

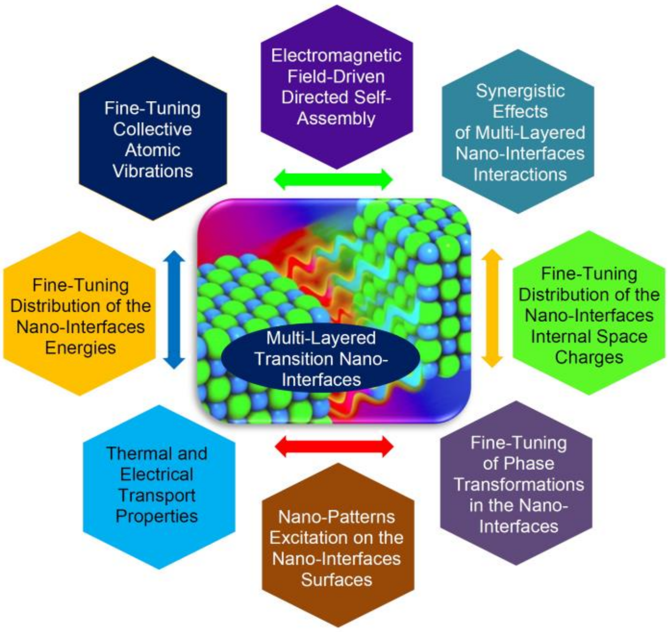

Figure 1. Refining the properties of artificially engineered multi-layered transition 3D-shaped nano-enhanced interfaces and maximizing their synergistic effects.

These interfaces are carefully fine-tuned using various effects and phenomena to achieve desired properties within the artificially structured multi-layered transition nano-enhanced interfaces.

Conclusion

We have introduced an original and innovative concept aimed at enhancing the efficiency of thermionic energy converters through the effective utilization of multilayer low-dimensional nano-carbon allotropes-based emitters. By implementing precise tuning of collective atomic vibrations, functionalities, and nanoarchitecture, we can reliably and predictably improve their performance. Our proposal involves leveraging the potential of 2D-ordered linear-chain carbon-based multilayered nano-enhanced interfaces to maximize their effectiveness and take advantage of their synergistic effects.

To achieve our goal of predictive excitation and adjustment within the nano-interface-based systems, and to harness the synergistic effects including collective atomic vibration synchronization, propagation of phonon waves, and efficient energy exchange within the multilayer carbyne-enriched 3D-shaped nano-enhanced interfaces, we have meticulously developed a comprehensive set of toolkits. These toolkits encompass an array of techniques, such as initiating allotropic phase transformations through energy-driven processes during simultaneous electron beam and ion irradiation, enabling precise control over the propagation of phonon waves. Additionally, we employ methods like micro/nano-manipulation using surface acoustic waves during ion-assisted pulse-plasma growth, combined with heteroatom doping, as well as directed self-assembly facilitated by external high-frequency electromagnetic fields. Furthermore, we adopt a data-driven carbon nanomaterials genome approach to guide our research endeavors.

This innovative approach sets the stage for the development of a new generation of thermionic energy conversion systems boasting significantly higher energy efficiency than their existing counterparts. The potential for surpassing the performance of current systems by several orders of magnitude is an exciting prospect.

Supplementary Materials: Presented poster. The material is available at the following link: https://static1.squarespace.com/static/5d078746ff1961000186c382/t/6458bc8fd3cf973751a3e027/1683537108465/SRW23-Posters.pdf.

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References

1. Go, D.; Haase, J.; George, M.J.; Wanke, R.; Nojeh A.; Nemanich R. Thermionic energy conversion in the twenty-first century: advances and opportunities for space and terrestrial applications. *Front. Mech. Eng.* **2017**, 3(13). https://doi.org/10.3389/fmech.2017.00013.
2. Campbell, M.; Celenza, T.; Schmitt, F.; Schwede, J.; Bargatin, I. Progress toward high power output in thermionic energy converters. *Adv. Sci.* **2021**, 8, 2003812. https://doi.org/10.1002/advs.202003812.
3. Paras; Yadav, K.; Kumar, P.; Teja, D.R.; Chakraborty, S.; Chakraborty, M.; Mohapatra, S.S.; Sahoo, A.; Chou, M.M.C.; Liang, C.-T.; et al. A Review on Low-Dimensional Nanomaterials: Nanofabrication, Characterization and Applications. *Nanomaterials* **2023**, 13, 160. https://doi.org/10.3390/nano13010160
4. Casari, C.S.; Milani, A. Carbyne: from the elusive allotrope to stable carbon atom wires. *MRS Commun.* **2018**, 8(2), 207-219. https://doi.org/10.1557/mrc.2018.48.
5. Flood, P.; Babaev, V.; Khvostov, V.; Novikov, N.; Guseva, M. Carbon material with a highly ordered linear-chain structure. In *Polyynes: Synthesis, Properties, and Applications*; Cataldo, F., Ed.; Taylor & Francis Group: Didcot, UK, **2005**; pp. 219–252. http://dx.doi.org/10.1201/9781420027587.ch11.
6. Gadre, C.A.; Yan, X.; Song, Q., et al. Nanoscale imaging of phonon dynamics by electron microscopy. *Nature* **2022**, 606, 292-299. https://doi.org/10.1038/s41586-022-04736-8.
7. Kumar, V.; Camden, J.P. Imaging vibrational excitations in the electron microscope. *Phys. Chem. C* **2022**, 126(40), 16919-16927. https://doi.org/10.1021/acs.jpcc.2c05108.
8. Hoglund, E.R.; Bao, D.L.; O'Hara, A., et al. Emergent interface vibrational structure of oxide superlattices. *Nature* **2022**, 601, 556-561. https://doi.org/10.1038/s41586-021-04238-z.