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Mathematically inspired structure design in nanoscale thermal transport

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Mathematically inspired structure design has emerged as a powerful approach for tailoring material properties, especially in nanoscale thermal transport, with promising applications both within this field and beyond. By employing mathematical principles, based on number theory, such as periodicity and quasi-periodic organizations, researchers have developed advanced structures with unique thermal behaviours. Although periodic phononic crystals have been extensively explored, various structural design methods based on alternative mathematical sequences have gained attention in recent years. This review provides an in-depth overview of these mathematical frameworks, focusing on nanoscale thermal transport. We examine key mathematical sequences, their foundational principles, and analyze the influence of thermal behavior, highlighting recent advancements in this field. Looking ahead, further exploration of mathematical sequences offers significant potential for the development of next-generation materials with tailored, multi-functional properties suited to diverse technological applications.

1 Introduction

The design of advanced materials has become increasingly crucial in the quest to enhance performance in a wide range of technological applications, from energy storage and electronics to thermal management systems[1–8]. A particularly critical challenge is the ability to control and optimize thermal transport properties, as effective thermal management directly impacts the efficiency and longevity of modern devices[9–11]. Beyond thermal transport, precise control of physical properties is also crucial in fields such as acoustic metamaterials[12–14], where sound manipulation is essential, and photonic crystals[15,16], which are fundamental to light propagation technologies. In this broader context, researchers have explored various approaches to tailor the material properties, with one emerging strategy being the integration of mathematical principles into material design.

The design of mathematics-inspired structures provides a versatile framework for manipulating various physical properties of materials. One of the most well-established approaches in this field is structural periodicity, which has been proven effective in modulating thermal and acoustic behavior. In the context of thermal transport, phononic crystals, which rely on periodic arrangements to influence phonon propagation, serve as a foundational model with a significant research history[6,17]. These structures have laid the groundwork for understanding how structure design can control thermal properties. Recently, however, researchers have begun exploring alternative mathematical sequences beyond simple periodicity, such as quasi-periodic and disordered structures. There is also some work based on the mathematical algorithms and graphic design[18], such as cyclotomic rule[19]. These emerging designs offer new possibilities for precisely tuning the behavior of materials at the nanoscale, opening up avenues for more sophisticated control over thermal and other physical properties.

Moving beyond simple periodic patterns, more intricate mathematical sequences, such as the Golomb ruler and Fibonacci sequences, introduce novel strategies for modulating thermal transport and various other physical properties. The non-redundant spacing of the Golomb ruler reduces phonon coherence, leading to phonon confinement and increased interface phonon scattering, thereby reducing thermal conductivity[20,21]. Similarly, the Fibonacci sequence, with its self-similar structure, facilitates the design of fractal-like architectures that reduce phonon coherence and manage heat dissipation across multiple scales, making it ideal for hierarchical thermal management in applications such as microelectronics[22]. Binary sequences composed of 0s and 1s, such as Thue-Morse and Double-Period[23], break translational symmetry while maintaining long-range order, effectively scattering phonons across a wide frequency range. This results in sig-

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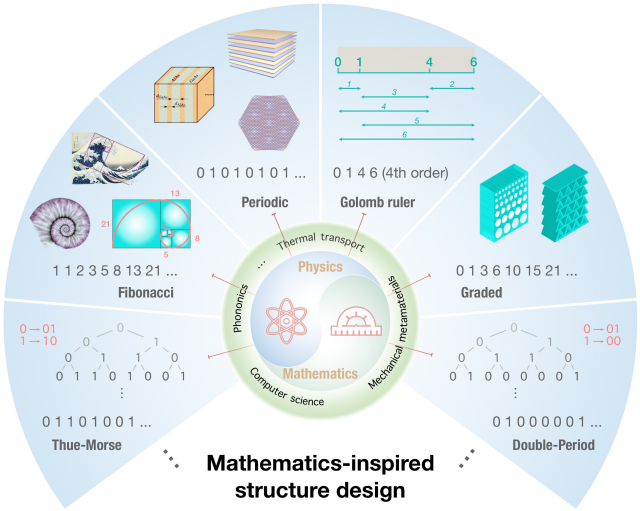

Fig. 1 Mathematics sequences for structure design in this review, from their generation principles to potential applications. The detail information of each sequence can be found in Sec. 2.

nificantly reduced thermal conductivity, making these structures well-suited for thermal barrier coatings in high-temperature environments such as aerospace and power generation, where decoupling thermal conductivity from mechanical strength is crucial. In addition, graded materials and hierarchical structures, inspired by natural systems, optimize thermal transport by creating gradual transitions in thermal conductivity and complex heat dissipation pathways, making them ideal for robust thermal management in energy systems and high-performance electronics[24].

This review aims to provide a comprehensive overview of the various mathematical frameworks based on number theory used in structure design, their effect on the thermal transport mechanisms of phonons, and the latest advances in their practical applications (Fig. 1). By integrating mathematical concepts with physical properties, we can achieve a level of control over material behavior that was previously unattainable, opening up new possibilities for the design of advanced materials with tailored functionalities. These advancements promise not only to boost fields like thermal management and energy conversion but also to pave the way for multifunctional materials that can meet the increasingly complex demands of modern technology.

2 Mathematical sequences for structural design

In this section, we list six typical mathematical sequences, respectively explaining their mathematical principles and characteristics used in structure design. To facilitate understanding, Fig. 2 uses simple two-dimensional (2D) graphene/hexagonal boron nitride (hBN)[22,23,25], graphene with isotope interfaces[21], and Si/Ge[24] systems as the model to show the structure design based on the various sequences mentioned above.

2.1 Period and superlattice

In solid-state physics and materials science, crystal and superlattice structures are essential concepts used to describe the periodic arrangement of atoms or molecules in solids. These structures can be mathematically characterized by their translation symmetry, exemplified by binary sequences such as 0, 1, 0, 1, 0, 1, 0, 1, and so forth, which dictate their periodicity and spatial configuration.

In a crystal, the position of each atom can be described by a combination of the primitive lattice vectors $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$ and a set of integers n_1, n_2, n_3, as given by the lattice vector: $\mathbf{R} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3$. The periodicity implies that any physical property $f(\mathbf{r})$ of the system satisfies the condition: $f(\mathbf{r}+\mathbf{R}) = f(\mathbf{r})$, for all lattice vectors $\mathbf{R}$ and positions $\mathbf{r}$ in the crystal. This translation invariance is the cornerstone of the Bloch theorem, which asserts that the electronic wave functions in a periodic potential can be expressed as Bloch functions, a product of a plane wave and a function with the same periodicity as the lattice. This underlying periodic order is responsible for many fundamental properties of materials, such as the formation of electronic band structures and the propagation of phonons.

A superlattice structure is a more complex form of periodicity resulting from the combination of two or more different materials, discovered by Johansson and Linde[26] in 1925. It can be thought of as a modulation of the original lattice structure, often achieved by alternating layers of different materials or varying the composition periodically. The superlattice is characterized by a longer periodicity, called the superlattice vector $\mathbf{R}_{SL}$, which can be expressed as: $\mathbf{R}_{SL} = m_1\mathbf{a}_1 + m_2\mathbf{a}_2 + m_3\mathbf{a}_3$, where m_1, m_2, and m_3 are integers that define the superlattice periodicity, typically larger than the primitive lattice vectors $\mathbf{a}_i$. This results in a larger unit cell for the superlattice compared to the underlying periodic structure.

Furthermore, this concept of introducing periodic modulation to manipulate material properties extends to other types of periodic structures such as phononic[12,27,28] and photonic[29–31] crystals. They expand the concept of periodic materials beyond superlattices, as they are not limited to two alternating materials, but can include a variety of structures such as arrays of holes, voids, or embedded inclusions[32–35]. These periodic configurations allow for precise control over the propagation of sound and light waves, creating band gaps that block specific frequencies. This broader versatility enables a wide range of applications, from acoustic insulation to advanced optical devices[36–39].

Periodic structures improve material properties by introducing an additional periodicity that modifies the fundamental characteristics of materials, such as the thermal[40–43], electronic[44,45], optical[46,47], and mechanical properties[48,49]. This structural complexity enables fine-tuning of material behavior beyond what is achievable in traditional crystals, making superlattices a versatile platform for exploring new physical phenomena and engineering advanced materials.

2.2 Golomb ruler

The Golomb ruler sequence was discovered by Sidon[50] and Babcock[51] independently and named for Solomon W. Golomb in first half of 20th century. Golomb rulers have since gained prominence in various mathematical and practical contexts due to their

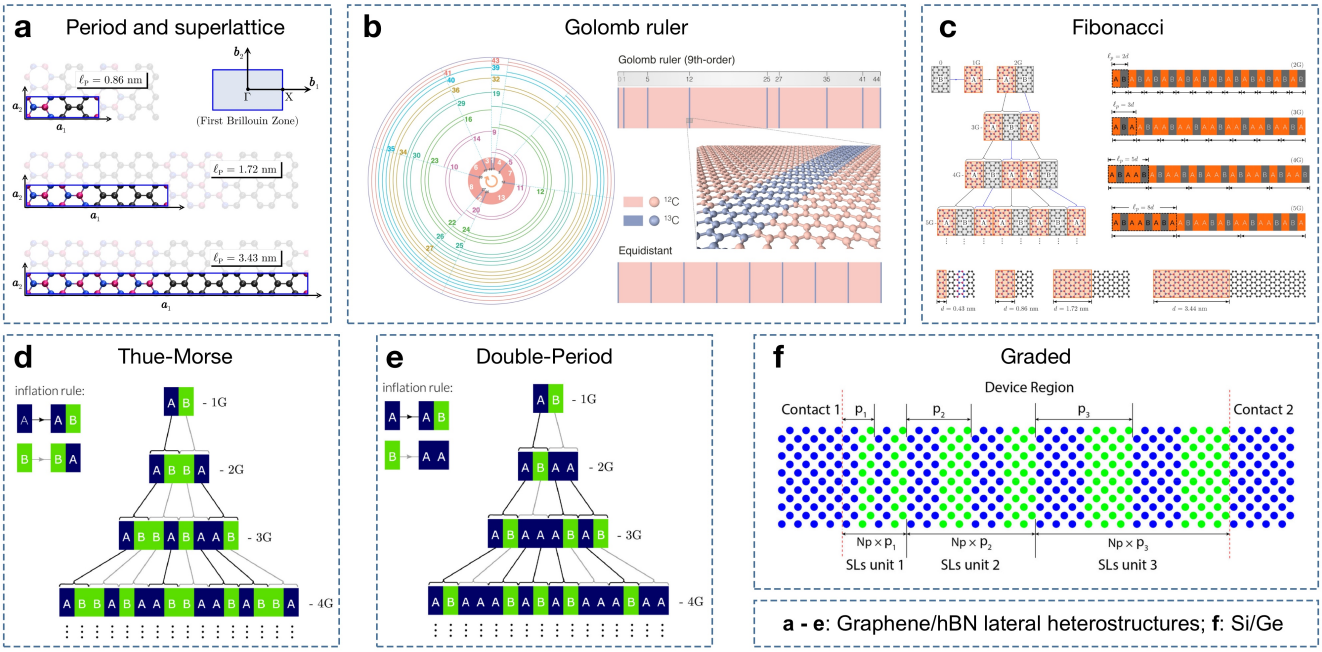

Fig. 2 Structure design cases based on 2D mathematical sequence applied in the field of nanoscale thermal transport. (a) Unitcell of graphene/hBN superlattices with increasing period length[25] (Copyright 2018, Springer Nature). (b) Graphene with isotope interfaces based on Golomb ruler sequences[21] (Copyright 2024, Elsevier). Graphene/hBN lateral heterostructures following the (c) Fibonacci[22] (Copyright 2020, Elsevier), (d) Thue-Morse[23] (Copyright 2022, Elsevier), and (e) Double Period[23] (Copyright 2022, Elsevier) sequences. (f) Schematic of the graded Si/Ge heterostructures[24] (Copyright 2021, AIP).

unique properties of non-redundant spacing.

A Golomb ruler is a sequence of marks at different positions along a ruler such that no two pairs of marks are the same distance apart[52–55]. Mathematically, an nth-order Golomb ruler with marks at positions m_1, m_2, …, m_n satisfies the condition that all pairwise distances $|m_i - m_j|$ for $1 \leq i < j \leq n$ are unique. The length of the Golomb ruler is defined as the distance between the smallest and largest mark, i.e., $m_n - m_1$. A Golomb ruler is not required to measure all distances up to its length. However, if it can do so, it is referred to as a perfect Golomb ruler. A Golomb ruler is considered optimal if no shorter ruler of the same order can be found. It has been proven that no perfect Golomb ruler exists for five or more marks, which means that all Golomb rulers of the fifth order and above are optimal.

Golomb rulers have versatile applications across various fields due to their unique property of non-redundant spacing. In communication systems, they are used to design error correction codes and synchronization sequences, minimizing signal interference[53]. In radio astronomy, the Golomb rulers optimize antenna array configurations, ensuring unique baseline measurements for better image resolution[51,56]. They also play a role in sensor placement for X-ray crystallography and seismic arrays, improving measurement accuracy by preventing redundant data collection[57]. Additionally, Golomb rulers are useful in network design and audio signal processing, where they help avoid interference and overlapping echoes, respectively[57]. Their broad applicability makes them valuable in any scenario requiring distinct and non-overlapping intervals.

2.3 Fibonacci

The Fibonacci sequence, named after the Italian mathematician Leonardo of Pisa (commonly known as Fibonacci), holds substantial historical and mathematical importance. Fibonacci introduced this sequence to the Western world in his 1202 book, Liber Abaci[58], where he used it to model the growth of an idealized rabbit population, illustrating the concept of exponential growth. However, this sequence was already well known in Indian mathematics long before Fibonacci's work, having been documented as early as 200 BCE in the context of Sanskrit prosody, where it was used to describe rhythmic patterns in poetry[59].

The Fibonacci sequence is defined by the recurrence relation $F(n) = F(n-1) + F(n-2)$ with initial conditions $F(0) = 0$ and $F(1) = 1$, generating a sequence that starts 0, 1, 1, 2, 3, 5, 8, 13, 21, and so on[60]. This simple yet powerful sequence is deeply intertwined with the golden ratio, as the ratio of successive Fibonacci numbers gradually converges to $\phi = \frac{1+\sqrt{5}}{2}$ as n approaches infinity. This convergence highlights the intrinsic connection between Fibonacci numbers and the golden ratio, reflecting the underlying harmony and aesthetic appeal that these mathematical concepts share.

The Fibonacci sequence finds diverse applications in several fields. In nature, it appears in the arrangement of leaves, flower petals, and seed heads, optimizing growth patterns and packing density[61]. In the realm of computer science, it serves as a fundamental example of recursion and dynamic programming, providing valuable insights for algorithm design[62]. Furthermore, the connection of the sequence to the golden ratio is of significance in art and architecture, where it supports aesthetically pleasing

proportions[63]. In general, the Fibonacci sequence is a remarkable mathematical construct that bridges the abstract and the concrete, finding expression in natural phenomena, human creativity, and sophisticated problem-solving frameworks. Its simplicity, coupled with its universality, renders it a persistent subject of scholarly interest, underscoring the profound interconnectedness of mathematics with the world around us.

2.4 Thue-Morse

The Thue-Morse sequence was first studied by Axel Thue in 1906 as part of his work on sequences that avoid repetitive patterns in the study of combinatorics on words. Later, in 1921, Marston Morse explored it further in the context of differential geometry and brought it to worldwide attention. It was originally developed to investigate sequences with complex structures that do not repeat in simple ways, laying the groundwork for areas like formal language theory and combinatorics.

The Thue-Morse sequence is an infinite binary sequence generated through a recursive process. It begins with $t_0 = 0$ and is constructed by successively appending the bitwise complement of the sequence obtained so far. The first few terms of this sequence are: 0, 01, 0110, 01101001, etc. Formally, the n-th term t_n of the sequence can be determined by examining the number of 1s in the binary representation of n: if the count of 1s is even, then $t_n = 0$; if odd, $t_n = 1$.

Alternatively, the Thue-Morse sequence can also be described using substitution rules, which reflect its inflationary nature. Starting with an initial element, 0, the sequence evolves by applying two simple substitution rules: $\phi(0) = 01$ and $\phi(1) = 10$. Thus, each occurrence of 0 in the sequence is replaced by "01" and each occurrence of 1 by "10". This recursive substitution process ensures that the sequence lacks repeating patterns and exhibits self-similarity, attributes that render it particularly useful for studies in combinatorics, computer science, and even physics.

Due to its non-repetitive, self-similar structure, Thue-Morse sequences have a range of applications. In computer science, it is used in algorithm design, digital signal processing, and error correction, as it helps minimize redundancy and interference[64]. In physics, the sequence is applied in the study of quasi-crystals and aperiodic tiling, providing insights into non-periodic structures[65–67]. These applications leverage the unique property of the sequence of avoiding consecutive identical patterns, which makes it valuable in various fields.

2.5 Double-Period

The Double-Period sequence represents a modified variation of the Thue-Morse sequence, distinguished by an alteration in its inflation rules. Rather than adhering to the standard Thue-Morse substitution rules, the Double-Period sequence is generated by the substitutions $\psi(0) = 01$ and $\psi(1) = 00$. Initiating from an initial element of 0, this process yields a sequence that evolves as follows: 0, 01, 0100, 01000101, and so forth.

The modified substitution rules produce a sequence with a more intricate and less balanced structure compared to the Thue-Morse sequence. Specifically, while the Thue-Morse sequence is known to avoid consecutive repetitions and maintain a high degree of self-similarity, the Double-Period sequence introduces frequent occurrences of '00' pairs. This alteration results in a sequence that diverges from the purely self-similar and non-repetitive characteristics of the Thue-Morse sequence, leading to a unique and less predictable pattern formation.

Due to these distinctive properties, the Double-Period sequence offers a valuable framework for exploring various nonperiodic patterns. Its irregular structure makes it an intriguing subject for research in fields such as coding theory, where its potential applications may include the design of error-correcting codes. In addition, the aperiodic nature of the sequence also holds promise for studies related to aperiodic structures and quasi-crystals, where non-repeating patterns play a significant role in understanding material properties and phenomena.

2.6 Graded

The graded sequence refers to a systematically controlled progression of material compositions in a specific direction, allowing deliberate adjustment of properties. These sequences can be engineered to follow various mathematical patterns, such as linear, exponential, or more complex functions, depending on the desired performance characteristics. This level of control offers a precise means of optimizing material properties across different regions of a structure.

A notable variant of graded sequences is found in functionally graded materials (FGMs). FGMs represent a class of advanced materials in which properties, such as composition, microstructure, mechanical strength, or thermal conductivity, vary continuously or in discrete steps over a particular dimension. This gradual variation enables these materials to provide a smooth and seamless transition between distinct phases or properties, effectively reducing issues related to material discontinuities, such as stress concentrations or thermal mismatches[68,69]. Using this unique capability, FGMs offers the potential for enhanced performance and customized functionalities that exceed those of traditional homogeneous materials. As a result, they are widely applied in industries that require high-performance materials with specialized properties, such as aerospace, electronics, and biomedical fields, where specific gradients in material properties can optimize their performance under various operating conditions[70,71].

3 Applications in nanoscale thermal transport

Mathematically inspired structure design offers a novel approach to optimizing material properties for various applications, particularly in nanoscale thermal transport. By applying mathematical principles, materials can be engineered with tailored functionalities that enhance performance in targeted areas. This section explores the application of these designs in nanoscale thermal transport within heterostructures, highlighting the potential for broader future applications across diverse fields.

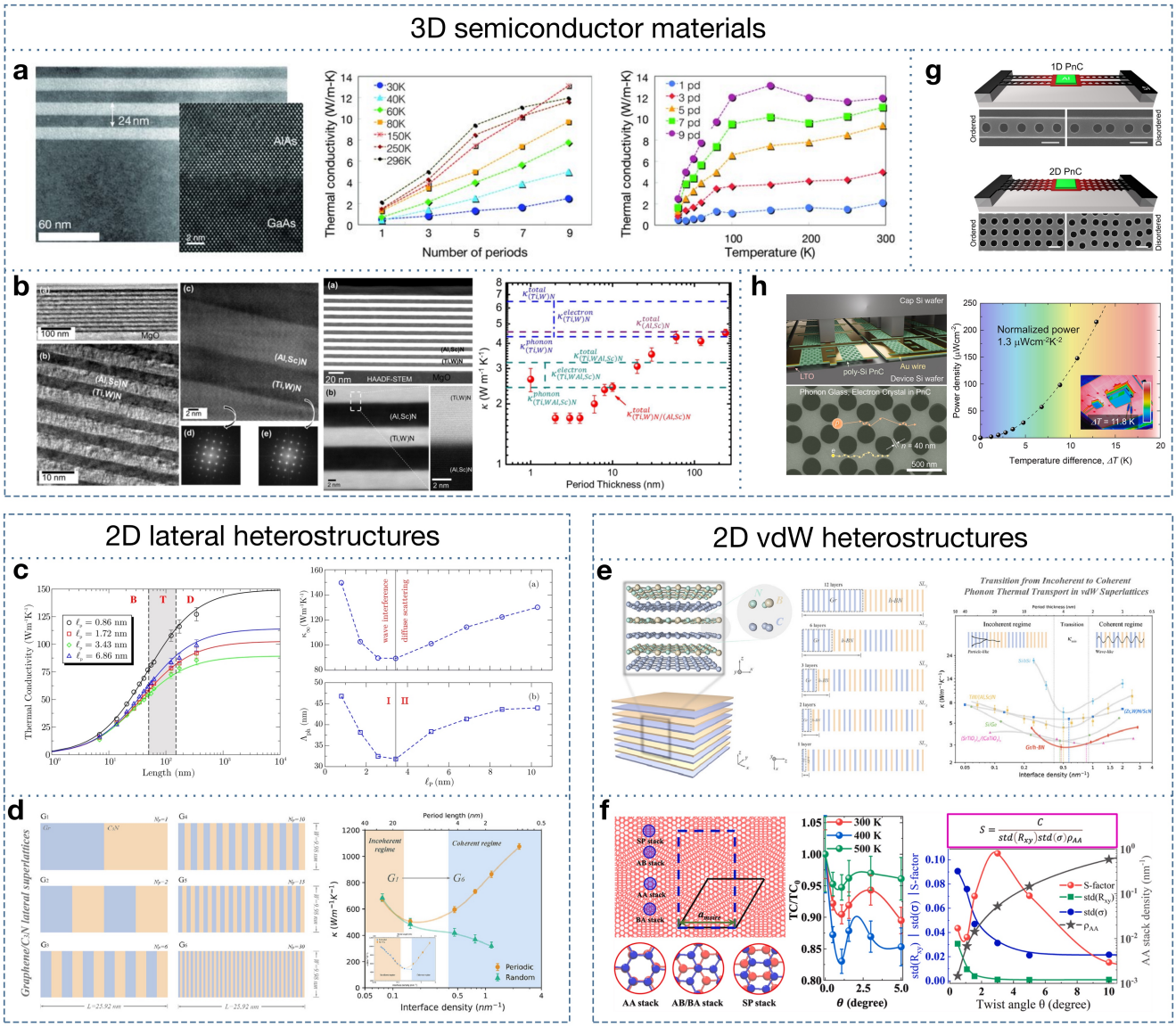

Fig. 3 The periodic structure design in the nanoscale thermal transport field. Experimental researches of phonon wave-particle crossover phenomenon in the (a) GaAs/AlAs[72] (Copyright 2012, AAAS) and (b) $Ti_{0.7}W_{0.3}N/Al_{0.72}Sc_{0.28}N$[73] (Copyright 2016, APS) three-dimensional (3D) semiconductor-based superlattices. Wave-particle crossover of phonon transport in the (c) graphene/hBN[25] (Copyright 2018, Springer Nature) and (d) graphene/2D polyaniline (C_3N) lateral superlattices[74] (Copyright 2023, Elsevier), and (e) graphene/hBN vdW superlattices[42] (Copyright 2022, Elsevier) via molecular dynamics (MD) simulations, which is the indication of transition in the phonon transport mechanism from the incoherent to coherent regime. (f) Thermal conductivity minimum of twisted bilayer graphene moiré superlattices[75] (Copyright 2023, Elsevier). (g) Schematic and SEM images show fabricated samples of one-dimensional (1D) and 2D phononic crystals (PnC) with ordered and disordered arrays of holes in silicon[76] (Copyright 2017, AAAS). (h) Enhancement of thermoelectric figure of merit by phononic nanostructure in silicon[77] (Copyright 2024, Elsevier).

3.1 Periodic

The periodic structure design in nanoscale thermal transport plays a crucial role in revealing the wave-particle crossover of phonon transport, where the phonon behavior transits between incoherent and coherent regime. The concept of minimum thermal conductivity in superlattices was first introduced by Simkin and Mahan[78] in 2000 through theoretical calculations, providing a foundation for understanding thermal behavior in these systems. Subsequent experimental investigations have validated the theoretical prediction. In GaAs/AlAs superlattices, the coherent phonon thermal transport process was experimentally confirmed for the first time by Luckyanova *et al.*[72], with measured thermal conductivity showing a linear increase as the total superlattice thickness increased over a temperature range of 30 to 150 K (Fig.3a). Similar observations have been made in epitaxial oxide $SrTiO_3/CaTiO_3$ superlattices, as reported by Ravichandran *et al.*[79], which provides experimental evidence of the transition from diffuse (particle-like) to specular (wave-like) phonon scattering. They directly observed the minimum in lattice thermal conductivity when varying the interface density. Moreover, Saha *et al.*[73] also demonstrated the phenomenon of phonon wave-particle crossover in (Ti,W) N/(Al,Sc) N metal/semiconductor su-

perlattices, grown epitaxially with periodicities from 1 to 240 nm. It revealed a delicate balance between long-wavelength coherent phonon modes and incoherent phonon scattering from heavy-tungsten atomic sites and superlattice interfaces. The ability to manipulate the transition from particle-like to wave-like phonon scattering by altering the superlattice design enables the optimization of thermal conductivity in various materials, offering a powerful platform for exploring phonon interference effects in superlattices with wide-ranging applications in thermoelectronics and thermal management.

Expanding on the foundational knowledge of phonon transport in periodic structures, recent studies on 2D materials and their heterostructures provide more profound insight into the wave-particle crossover phenomenon. For the 2D lateral heterostructures, in the graphene/hBN case, MD simulations conducted by Felix and Pereira [23] clearly demonstrated this crossover, as phonon transport evolves from a particle-to-wave-like mechanism (Fig.3c). This phenomenon is similarly observed in graphene/2D polyaniline (C_3N) lateral superlattices, where the dual effect of the heterointerface mechanism identified by Wu *et al.* [74] further supports the understanding of the behavior of phonons at nanoscale interfaces (Fig.3d). The gradual transition from incoherent scattering to coherent wave propagation in these systems is governed by the interplay of superlattice periodicity and material properties, which directly affects thermal conductivity. For the 2D van der Waals (vdW) heterostructures, Wu and Han [42] extended this analysis by showcasing how the layered nature of graphene/hBN vdW superlattices leads to a transition in phonon transport regimes (Fig.3e). As the period thickness decreases, the phonon transport shifts toward coherence, significantly affecting the thermal conductivity. These insights underscore the potential for the tuning of thermal properties in layered 2D systems, opening possibilities for advanced thermal management in nano devices. Additionally, Cheng *et al.* [75] demonstrated that in twisted bilayer graphene moiré superlattices, which are unique periodic structures formed by the slight rotational misalignment of two graphene layers, the twist angle plays a critical role in determining phonon transport (Fig.3f). This specific arrangement induces a moiré pattern that creates periodic potential landscapes, significantly affecting both electronic and phononic properties [80–82]. At specific magic angles, a minimum in thermal conductivity was observed as a result of enhanced phonon scattering and interference, further reinforcing the intricate relationship between lattice structure and phonon dynamics.

In addition to 2D materials, silicon-based structures represent a significant area of interest in thermal transport research. Silicon, widely used in electronics and thermoelectric devices, serves as an ideal platform for exploring phonon transport manipulation. The work of Maire *et al.* [76] demonstrated the successful fabrication of 1D and 2D PnC in silicon, with ordered and disordered arrays of holes (Fig. 3g). The comparison of these structures shows how phonon transport can be tailored through periodicity and disorder, offering valuable insights for thermal management strategies in silicon-based devices. Furthermore, PnC also offers promising approaches to improve thermoelectric performance, as shown by Yanagisawa *et al.* [77] (Fig. 3h). By introducing periodic nanostructures in silicon, phonon scattering is significantly enhanced, resulting in a reduction of thermal conductivity while preserving electrical properties. This modification boosts the thermoelectric figure of merit, facilitating a ten-fold improvement in power generation efficiency. Consequently, this advancement enables once-a-day sensing applications to become feasible in practical environments, marking a critical step forward in energy harvesting technologies.

This comprehensive exploration of phonon transport mechanisms across different material systems underscores the importance of periodic structure design in manipulating the thermal properties at the nanoscale. The combined insights from simulation, theoretical analysis, and experimental validation highlight the potential to advance thermal management and thermoelectric applications through controlled phonon transport.

3.2 Quasi-periodic and disordered

In the field of nanoscale thermal transport, quasiperiodic and disordered structure designs, particularly in 2D materials, have shown promising potential to modulate thermal conductivity. The exploration of such designs, inspired by mathematical sequences, aims to understand and control phonon transport behaviors within these materials. This is especially pertinent for applications requiring precise thermal management, such as thermoelectric devices and heat dissipation technologies.

One prominent approach is the quasi-periodic arrangement of graphene/hBN lateral heterostructures, utilizing sequences such as Fibonacci, Thue–Morse, and Double-Period to create a variety of configurations (Fig. 4a). Specifically, the research from Felix and Pereira [22] indicated that quasiperiodicity of Fibonacci sequences in graphene/hBN heterostructures suppresses coherent phonon transport by increasing interface density as Fibonacci generation increases, disrupting phonon coherence. This effect enhances nanoscale control over thermal transport, suggesting potential for advanced thermal management device applications. They also explored phonon transport in graphene/hBN superlattices with Thue–Morse and Double-Period sequences [23], finding that high generations suppress coherent thermal transport similarly to Fibonacci-based structures. The suppression is caused by an increase in the superlattice period (or quasi-periodic generation), which can lead to phonon localization with some certain wavelengths, reducing the lattice thermal conductivity. However, whether it is the Fibonacci, Thue-Morse, or Double-Period sequences, their effectiveness in suppressing phonon thermal transport remains limited because of their inherent periodicity.

To achieve more effective suppression of thermal conductivity, Wu *et al.* [20] reported a more disordered structure design based on the fifth order Golomb ruler sequence in graphene/hBN heterostructures (Fig. 4b). This design introduces greater diversity and irregularity in the interface spacing, enabling a wider range of phonon wavelengths to be suppressed. This sequence has shown potential for reducing the thermal conductivity by increasing the interface density, which is a valuable feature for applications requiring thermal insulation. Furthermore, they extended it to graphene nanoribbons with ^{13}C isotope interfaces,

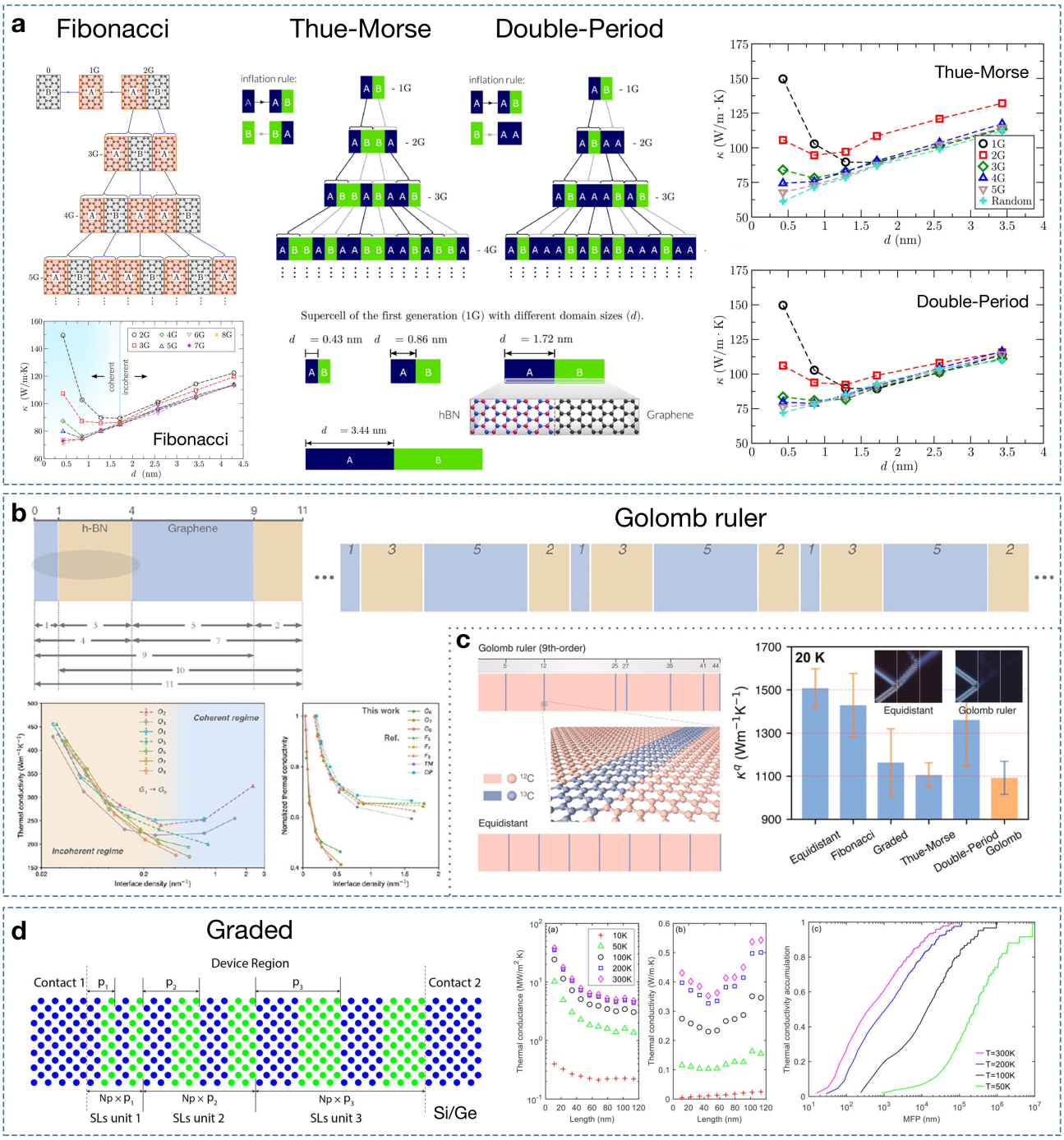

Fig. 4 The quasi-periodic and disordered structure design in the nanoscale thermal transport. (a) Quasi-periodic generations for Fibonacci, Thue–Morse, and Double-Period sequences, and the intrinsic thermal conductivity versus domain sizes of sequenced graphene/hBN lateral heterostructures [22,23] (Copyright 2020, Elsevier). (b) Graphene/hBN lateral heterostructures based on the 5th-order Golomb ruler sequence and their thermal conductivity with different interface densities [20] (Copyright 2023, Elsevier). (c) Graphene nanoribbon with ^{13}C isotope interfaces based on the 9th-order Golomb ruler sequence, and its thermal conductivity compared with other mathematical sequences at 20 K [21] (Copyright 2024, Elsevier). (d) Phonon localization in graded Si/Ge superlattices [24]. (Copyright 2021, AIP)

utilizing a 9th-order Golomb ruler sequence to manage thermal properties at cryogenic temperatures [21] (Fig. 4c). They found that the specific arrangement of these isotope interfaces notably suppresses thermal transport at 20 K, illustrating how isotope engineering in combination with mathematical sequences can effectively modulate phonon transport over a broader range of wavelengths in cryogenic environments. The Golomb ruler sequence stands out for its ability to disrupt phonon coherence through irregular spacing, enabling the suppression of a wide range of phonon wavelengths. Unlike random sequences, the Golomb

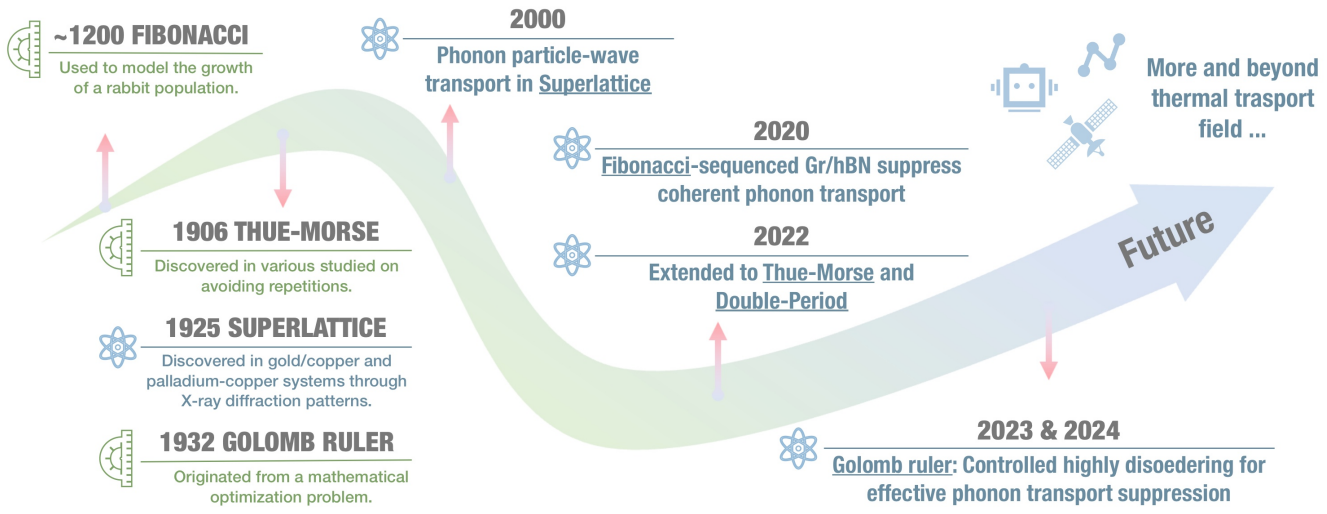

Fig. 5 The timeline of the discovery of the mathematical sequences in this review and their applications in nanoscale thermal transport field.

ruler sequence provides a structured form of strong disorder that is both predictable and mathematically defined. This sequence offers a controlled irregularity, allowing researchers to precisely design systems with known spacing irregularities. By employing the Golomb ruler sequence, one can achieve a consistent, repeatable pattern of disorder, offering a unique approach to modulating thermal conductivity and other transport properties with greater control than purely random arrangements allow.

Additionally, recent studies have also explored innovative methods to manipulate phonon behavior in Si/Ge superlattices, aiming to enhance thermal control through graded-based interfaces. Guo *et al.* [24] introduced a novel approach to phonon localization in graded Si/Ge superlattices, showing that a sufficient level of long-range disorder can lead to a thermal conductivity minimum by partially localizing moderate-frequency phonons (Fig. 4d). By analyzing length-dependent transmission and participation ratios, as well as phonon density distributions, the work highlights a unique regime where phonon transmission decays exponentially, offering new insights into phonon localization and thermal conduction engineering through wave-based phonon control. Ma *et al.* [83] studied the thermal conduction phenomena and phonon spectrum characteristics of interfaces with graded Si/Ge system. Compared with linearly varying mass gradient layers, as well as uniform mass layers and pure Si/Ge interfaces, the exponentially varying mass gradient model has more phonons that can be transmitted across adjacent layers, resulting in significant improvement of interface thermal conductance.

As above, by incorporating non-periodic sequences, researchers have developed materials that effectively modulate heat conduction through tailored phonon scattering mechanisms. These approaches demonstrate the potential of mathematical sequences to enhance thermal management in advanced material applications, offering new pathways for modulating nanoscale thermal transport.

4 Conclusions and outlook

This review has summarized recent advancements in controlling nanoscale thermal transport through the design of mathematically inspired structures, such as superlattices and quasi-periodic frameworks. While classical mathematical sequences have been studied for nearly a century, it is only in the 21st century that they have inspired novel approaches to physical structure optimization, marking a fresh perspective in the field (Fig. 5). These designs deepen our understanding of nanoscale thermal transport physics, showing substantial promise for manipulating thermal conductivity and more applications by enabling precise control over thermal transport mechanisms. With this in mind, we propose the following outlook:

While recent machine learning (ML)-driven approaches have produced innovative designs for nanoscale thermal transport [84–88], they often rely on data-intensive optimization and rule-based selection processes. However, although these methods are highly effective, their results often lack strong predictability and clear definition. Mathematical principles, on the contrary, offer clearer and direct insights, though they may not achieve the same high optimization level. Looking ahead, integrating mathematical approaches with ML could unlock new possibilities in thermal management, energy harvesting, and advanced material development. Furthermore, mathematical methods can be considered to guide intrinsic thermal nonlinearity for more efficient heat harvesting, as discussed by Zhou *et al.* [89]. By combining the intuitive clarity of mathematical designs with the optimization strength of ML, we could harness the strengths of both methods to refine and enhance the thermal transport properties.

Mathematical sequence-inspired designs offer promising guidance for experimental studies in thermal transport, providing a structured approach to controlling heat flow at the nanoscale. Although simulations reveal the potential of these designs, directly translating them to experimental scales is challenging. Despite this, simulations still offer valuable insight that can guide and inspire the creation of similar designs in experimental settings.

By bridging simulation insights with practical applications, these frameworks can deepen our understanding of complex heat conduction behaviors and drive advancements in advanced thermal management and thermal design systems.

Furthermore, mathematically inspired structure design methods hold potential for broader applications beyond thermal transport control. These principles could drive advances in fields such as energy harvesting, signal processing, and wave manipulation, where precise control over material properties is crucial. By enabling adaptable, scale-sensitive designs, mathematical sequences provide pathways for creating materials with tunable behaviors to meet diverse functional requirements. As computational methods continue to evolve, these designs may foster breakthroughs in the optimization of complex material systems in various scientific and engineering disciplines.

Conflicts of interest

There are no conflicts to declare.

Data availability

No new data were generated or analyzed as part of this review.

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Data availability

No new data were generated or analyzed as part of this review.