

# Review of coherent phonon and heat transport control in one-dimensional phononic crystals at nanoscale <sup>EP</sup>

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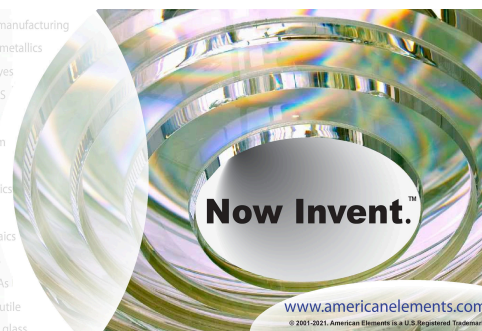
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## ABSTRACT

Phononic crystals are the acoustic analogs of photonic crystals and aim at manipulating phonon transport using phonon interference in periodic structures. While such periodic structures are typically two-dimensional, many applications require one-dimensional (1D) wire-like or bulk structures instead. In this Research Update, we summarize the past decade of theoretical and experimental studies of coherent control of phonon and heat transport in one-dimensional phononic crystals. At the hypersonic frequencies, phononic crystals successfully found applications in optomechanical devices at the microscale. However, at higher terahertz frequencies, experimentalists struggle to demonstrate that coherent thermal transport at room temperature is possible at length scales of hundreds of nanometers. Although many theoretical works predict a reduction in the thermal conductivity in 1D phononic crystals due to coherent effects, most observations conclude about the incoherent nature of heat conduction at least at room temperature. Nevertheless, experiments on superlattices and carbon nanotubes have demonstrated evidence of coherent heat conduction even at room temperature in structures with the periodicity of a few nanometers. Thus, further miniaturization and improving fabrication quality are currently the main challenges faced by 1D phononic nanostructures.

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## INTRODUCTION

Phonons are the primary carriers of sound, heat, and mechanical vibrations in semiconductors. Thus, controlling phonon transport has always been one of the primary goals for researchers working on thermoelectric, electromechanical, and optomechanical systems. Being inspired by light manipulations based on the wave interference of photons,<sup>1,2</sup> researchers applied a similar approach to manipulations of phonons, as phonons are essentially waves in the atomic lattice.

This wave-based approach led to the development of acoustic analogs of photonic crystals called phononic crystals<sup>3–5</sup>—the artificial structures with periodic boundaries that systematically reflect phonons and cause phonon interference. Ever since, phononic crystals have been gradually decreasing in size from the micro- to

nanoscale, thus increasing the frequency of phonons they could affect and potentially control.<sup>6–8</sup>

Today, two-dimensional (2D) phononic crystals became an alternative component in various systems, including optomechanical cavities,<sup>9,10</sup> sensors,<sup>11,12</sup> and thermoelectric generators.<sup>13,14</sup> However, advances in nanowire fabrication, electron-beam lithography, and molecular beam epitaxy motivated the use of one-dimensional (1D) structures as a base for future phononic devices.<sup>15–18</sup> Subsequently, 1D phononic crystals emerged as an enhancement of 1D wires, beams, and bulk materials with applications at ultrasonic, hypersonic, and even terahertz frequencies.

This Research Update summarizes the past decade of studies on the coherent transport of phonons and heat in 1D phononic structures. First, we illustrate the basic principles of coherent control of phonon dispersion in 1D phononic structures. Next, we review

studies using coherent control to enhance the optomechanical coupling of low-frequency phonons in optomechanical systems. Then, we summarize recent theoretical and experimental works using 1D phononic crystals for controlling high-frequency phonons and heat. Finally, we overview the success in the experimental demonstration of coherent heat conduction at room temperature in the superlattices.

## PHONON DISPERSION ENGINEERING

The key mechanism enabling control over the phonon transport in phononic crystals is the phonon wave interference caused by the additional periodic scatterers. The interference occurs only when phonons systematically reflect from periodic boundaries preserving their phase or, in other words, staying coherent. For this reason, this approach and its resulting effects are often labeled as coherent. The interference changes the phonon dispersion, which affects the phonon properties of the structure, including phonon group velocity and density of states.<sup>19,20</sup> The dispersion changes may include flattening of the bands and formation of bandgaps—ranges of frequency in which phonons cannot propagate.<sup>21</sup>

Figure 1 illustrates how the addition of periodic wings to a nanowire causes substantial flattening of the dispersion branches and occurrence of the bandgaps.<sup>22</sup> In such nanostructures with additional wings or pillars, researchers distinguish two types of phonon interference: the interference caused by the periodicity of the scatterers and the local resonances inside the scatterers due to the presence of resonant modes.<sup>7,23</sup>

To illustrate this distinction, the color of the dispersion branches reflects the physical location of the average displacement  $\xi$ , with brighter color representing the displacement located closer to the nanowire and darker color representing the displacement deeper in wings. Indeed, the modes next to the eigenfrequencies of the wings tend to be flat and dark, indicating the states localized in the wings, whereas the rest of the modes tend to be bright and not flat. To further visualize, Figs. 1(c) and 1(d) show the calculated displacement fields for the branches affected by the interference caused by periodicity and by local resonances in the wing.<sup>7</sup>

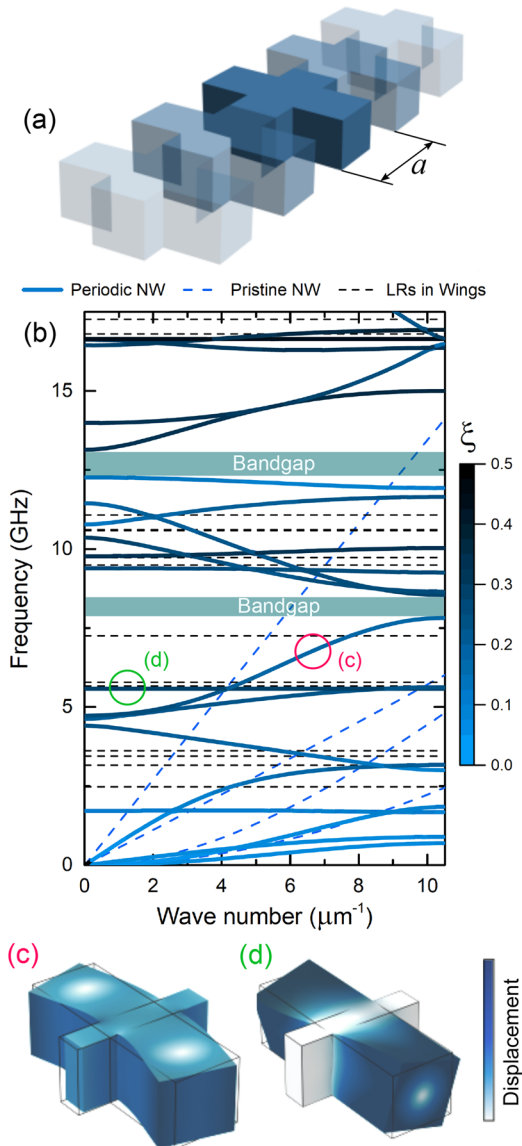
Thus, both the periodicity of the wings and their size can be used to tune the phonon dispersion of the structure, which enables the adjustment of both the frequency and the size of acoustic bandgaps.<sup>23</sup> In the next two sections, we show how such tuning enables designing complex optomechanical systems and reducing the overall thermal conductivity of nanostructures.

## PHONON CONFINEMENT FOR OPTOMECHANICS

Optomechanics is based on optomechanical (OM) coupling—the interaction between the electromagnetic field and vibrational modes of matter. Applications of optomechanics include mass and motion sensing, such as in the Laser Interferometer Gravitational-Wave Observatory (LIGO) gravitational wave detector, and communication, including quantum computation using phonons. Here, we focus on a specific class of OM structures—the 1D OM crystals.

The OM crystals essentially combine both photonic and phononic crystals in which the electromagnetic and mechanical

waves are co-localized to enhance their coupling.<sup>17,26–30</sup> The co-localization occurs due to a defect (cavity) in the otherwise periodic modulation of the refractive index and material density. The frequency of the confined optical and mechanical modes lies inside the photonic and phononic bandgaps, respectively. Since no mode can exist within the bandgaps of perfect media, a defect allows creating a cavity mode. Such a defect is usually implemented by inserting a region between the Bragg mirrors in which the periodicity is broken.



**FIG. 1.** (a) Scheme of a periodic 1D phononic crystal and (b) its phonon dispersion showing the formation of acoustic bandgaps and flattening of dispersion branches.<sup>22</sup> The color of the dispersion branches indicates the physical location of the average displacement field, with blue color representing displacement in the center of the beam and dark color representing the displacement in the wings. (c) and (d) Simulated displacement field corresponding to modes indicated in (b).

Figure 2(a) shows an example of an OM crystal consisting of a nanobeam with a periodic array of holes and side fins. In the center of the beam, the periodicity is gradually reduced, creating both optical and mechanical cavities surrounded by the periodic regions functioning as Bragg mirrors.

The confined photonic modes are often designed to have the telecommunication wavelength ( $\lambda \approx 1500$  nm) due to the ease of coupling with waveguides and optical fibers. Indeed, the laser wavelength is adjusted to match one of the resonant modes of the undeformed cavity, which satisfies the condition of a standing wave:  $\lambda_n = 2L_{\text{eff}}/n$ , where  $L_{\text{eff}}$  is the effective length of the cavity and  $n$  is an integer number. The light in the cavity then exerts radiation pressure force on the Bragg mirrors, thus deforming the cavity by changing its effective length, which is especially efficient for small structures and high-intensity fields in the cavity. The cavity length and stress distribution are then modified, which creates a feedback loop that alters the radiation pressure force, again moving the mirrors.

The optical properties, including the optical resonances, thus depend on the mechanical motion.<sup>9,24</sup> Similarly, such a cavity possesses mechanical resonances that can be tuned to the desired frequencies in the MHz–GHz range. The mechanical motion is affected by the optical field due to the radiation pressure force. This double coupling constitutes the key point of cavity optomechanics, and the OM interaction can therefore amplify or dampen the mechanical motion. Moreover, optical cavity resonances can also be coupled either to mechanical cavity modes or, in the case of nanobeams, to string modes of the entire beam.

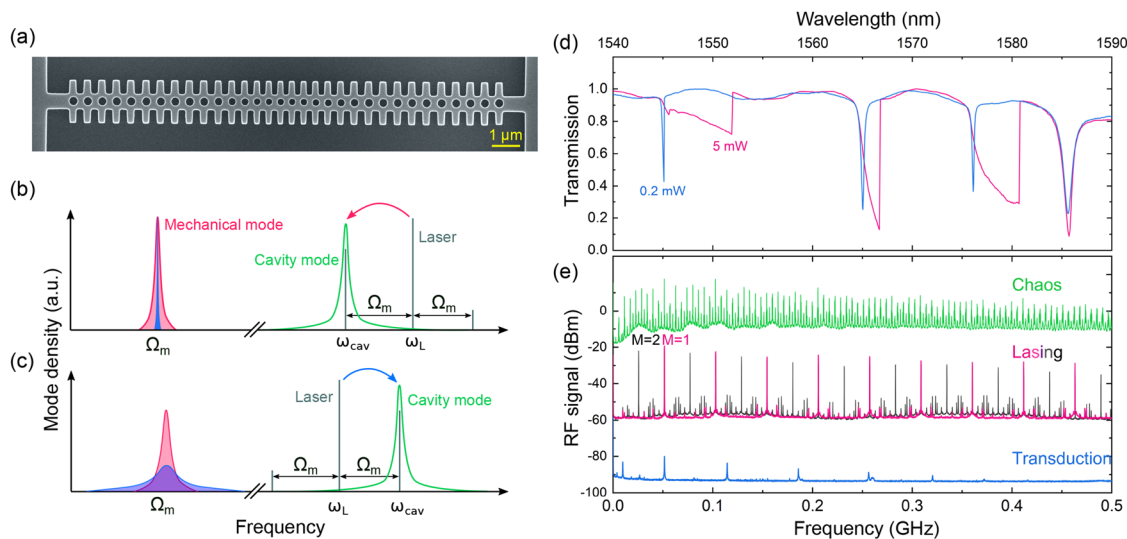
In OM crystals, controlling self-sustained high-amplitude coherent oscillations has been one of the most investigated subjects.

This regime, often called phonon lasing, can be achieved with different strategies, including dynamical backaction and self-pulsing.

In the case of the dynamical backaction, the phonon lasing regime is achieved by compensation of the intrinsic mechanical losses. If the optical decay rate is lower than the mechanical frequency, then an OM cavity is considered to be in the sideband-resolved regime. In this regime, the optical cavity cannot instantaneously react to the change in geometry due to the mechanical motion. The radiation force acquires an out-of-phase component, and therefore, a net phase delay appears. During one cycle of mechanical oscillation, the work of radiation force can be either negative or positive when the laser is detuned from the resonance to lower or higher frequencies. These two regimes correspond to the damping and amplification of the mechanical motion [Figs. 2(b) and 2(c)], with the latter enabling phonon lasing.

Achieving the maximum of damping or amplification requires pumping of the cavity by a laser detuned from the optical resonance by a frequency corresponding to the mechanical frequency  $\Omega_m$ , as shown in Figs. 2(b) and 2(c). A complete mathematical derivation is given by Aspelmeyer *et al.*<sup>24</sup>

Another strategy to induce phonon lasing is the self-pulsing mechanism. The example structure, given in Fig. 2(a), is designed to have a photonic pseudogap at the wavelength of 1550 nm and a complete phononic bandgap<sup>17</sup> unlike most structures found in the literature.<sup>27,31,32</sup> Characterization is often performed using near-field coupling via fiber optics where the light intensity emitted by an infrared laser and transmitted through the fiber is measured. Figure 2(d) shows the measured transmission spectrum. At low input power ( $<0.2$  mW), the spectrum displays dips corresponding



**FIG. 2.** (a) Scanning electron microscopy (SEM) image of the OMC nanobeam. A schematic principle of mechanical amplification (b) and damping (c) in an OM cavity is shown.<sup>24</sup> When the pump laser is detuned from the optical resonance by the frequency of the mechanical motion  $\Omega_m$  and  $-\Omega_m$ , the imbalance between Stokes and anti-Stokes scattering leads to mechanical amplification or damping, respectively. (d) Normalized spectra of the optical transmission obtained at low (blue) and high (red) power. In the low power transmission spectrum, optical resonances appear as sharp symmetrical dips. When the laser power is high enough to heat the cavity, the shape of the resonances becomes asymmetric, which is characteristic of the thermo-optic effect. (e) Mechanical spectra for three different regimes of the OM cavity. In the transduction of thermally activated modes (blue) the amplitude of the peaks is low. In the phonon lasing due to the first and second harmonics of the optical force (red and black curves, respectively), the amplitude increases and harmonics become clearly visible. In the chaos regime (green), phonon lasing still occurs but the optical signal is chaotic. Transduction, phonon lasing and chaos are shown from bottom to top, respectively. (d) and (e).

to the high-quality factor resonances that match the localized optical modes of the OM crystal. Indeed, the low-frequency peaks that appear in the RF spectrum correspond to the transduction of the thermally activated in-plane and out-of-plane string modes of the nanobeams [Fig. 2(e)]. The OM coupling between these modes and the electromagnetic field is strongly enhanced due to fabrication-induced asymmetry of the nanobeam with respect to its width, without which it would be negligible. The third order in-plane eigenmode, shown in Fig. 2(e), has been extensively used to investigate non-linear dynamics in these structures.

The self-pulsing frequencies can vary depending on the system from a few mHz in SiN microdisks<sup>39</sup> to a few tens of MHz in the nanobeam described here and up to several hundreds of MHz for an integer multiple of the fundamental frequency.<sup>40</sup> When the self-pulsing frequency equals an integer multiple of the mechanical resonator frequency, the system reaches self-sustained mechanical oscillations that are of high amplitude and coherent, as shown in Fig. 2(e), thus satisfying the requirements for a phonon lasing state.<sup>40</sup>

Other regimes can be achieved with this scheme, such as period doubling and chaos<sup>30</sup> [Fig. 2(e)], which is of particular interest for cryptography. Remarkably, this system can also be used to dynamically switch between these oscillation regimes<sup>25</sup> or to synchronize several OM cavities.<sup>41</sup> A combination of both phenomena enables a dynamic synchronization switch. The interest in synchronization, which is a pervasive phenomenon in nature,<sup>42–46</sup> lies in its many applications in timekeeping, sensors with low phase noise, and neural networks.

Beyond phonon lasing, notable effects have been achieved in similar OM structures: for example, laser cooling below the ground state, meaning that the average phonon population of the cavity is below one, or optical combs.<sup>31</sup> Another strategy has recently been proposed in 1D OM structures, which is the use of Anderson localization to confine phonon modes in aperiodic superlattice pillars or nanobeams with fabrication imperfections.<sup>47,48</sup> This approach can have advantages in terms of frequency and mode volume. Taking advantage of rapid progress in nanofabrication, this field of study is progressing toward optomechanical circuits and quantum applications.<sup>49</sup>

## COHERENT HEAT CONDUCTION IN 1D BEAMS

Success in coherent control of low-frequency phonons in optomechanics motivated researchers to explore the use of 1D phononic nanostructures for controlling higher-frequency phonons. Since heat in semiconductors is primarily carried by high-frequency “thermal” phonons, the coherent control over these phonons may ultimately lead to the control over heat conduction. Thus, the regime in which phonons that carry thermal energy stay coherent is called coherent heat conduction.

Theoretical studies predicted that the addition of periodic wings (pillars)<sup>22,50–52</sup> or walls (diameter modulations)<sup>50,53–55</sup> to pristine nanowires and nanowire corrugation<sup>56</sup> should substantially reduce the thermal conductivity. A recent review by Jin *et al.*<sup>57</sup> explains in detail the coherent control of heat conduction via nanopillars.

As a rule, the reduction grows with the size of the wings since larger wings cause stronger modifications to phonon dispersion. These stronger dispersion modifications originate from both the

larger number of local resonant modes<sup>58,59</sup> and stronger impact of the periodicity.<sup>60</sup> For similar reasons, the thermal conductivity becomes even lower if wings are present on multiple sides of the wire.<sup>50,52,58</sup>

However, any additions to pristine nanowires also introduce additional incoherent (diffuse) phonon surface scattering,<sup>51</sup> leading to the reduction in the phonon mean free path.<sup>50</sup> Thus, the reduction in the thermal conductivity observed in simulations may originate from both coherent modifications of phonon dispersion and incoherent surface scattering of phonons. Ma *et al.*<sup>51</sup> tried to separate the coherent and incoherent impacts of the wings by performing both Monte Carlo and atomistic simulations of the same 1D periodic structures. They found that 38% of the total thermal conductivity reduction is caused by incoherent mechanisms. Likewise, other Monte Carlo simulations under particle approximation<sup>35,61–63</sup> demonstrated that about 20% reduction in the thermal conductivity could be explained by incoherent scattering.

Moreover, finite element method (FEM) simulations,<sup>25</sup> which take into account neither coherent nor incoherent effects, showed that about 10% of the thermal conductance is reduced by the wings simply due to their additional material volume and corresponding extension of the heat flux lines.

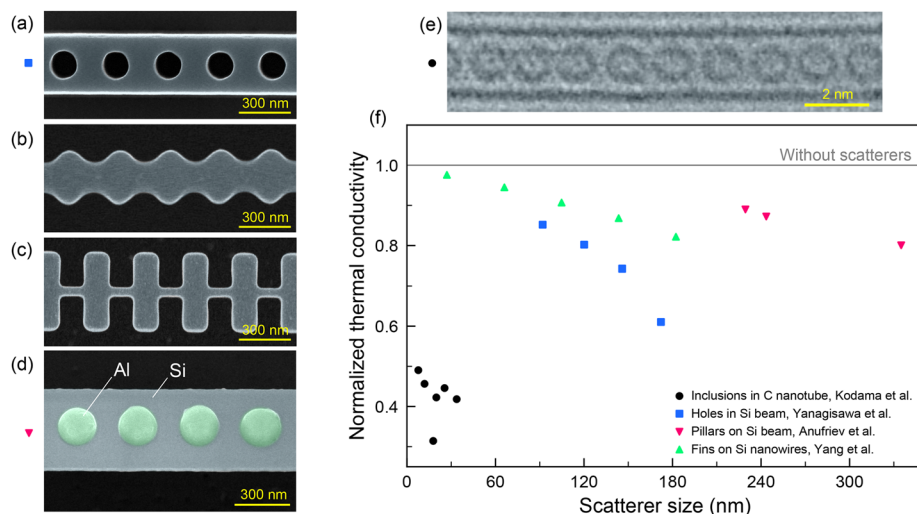
Many attempts to experimentally confirm the theoretical predictions have been reported over the past decade. The measurement on silicon nanowires at room temperature<sup>25,38</sup> could indeed detect an 18% reduction of the thermal conductivity due to the addition of periodic wings, shown in Fig. 3. The observed reduction was explained by incoherent diffuse surface scattering and added constriction resistance without invoking any coherent effects.

Experiments on corrugated silicon nanowires [Fig. 3(b)] also demonstrated a reduction in thermal conductivity due to the corrugation of pristine nanowires.<sup>34,67,68</sup> Poborchii *et al.*<sup>67</sup> attributed the observed reduction to the reduced group velocity caused by coherent modifications of phonon dispersion. However, the phonon interference seems to be an unlikely reason for the observed reduction regarding the high surface roughness of the samples and room temperature of the experiment. On the other hand, Blanc *et al.*<sup>68</sup> and Anufriev *et al.*<sup>34</sup> explained the observed reduction by diffuse scattering of phonons on the corrugated surfaces, even taking into account much lower surface roughness and low temperatures of their experiments.

In addition to nanowires with periodic modifications, many experiments focused on another type of phononic crystal consisting of a beam with arrays of holes with a period of a few hundred nanometers,<sup>14,33,69,70</sup> as shown in Fig. 3(a). Early experiments at room temperature<sup>14,69,70</sup> demonstrated that holes reduce the thermal conductivity of the beam proportionally to the hole diameter [Fig. 3(f)] and hole surface roughness. This reduction was explained in terms of the Callaway–Holland model by incoherent phonon scattering on holes. Marconnet *et al.*<sup>69</sup> estimated that coherent effects in such phononic structures should only occur at temperatures below 10 K.

To verify this prediction, Maire *et al.*<sup>33</sup> measured the same nanobeams with ordered and disordered arrays of holes at low temperatures. They found that at 4 K, an ordered array of holes reduces the thermal conductivity by 8% more than disordered arrays. This dependence on the hole order was interpreted as a fingerprint of coherent effects since phonon interference should be weaker





**FIG. 3.** SEM images of various 1D phononic crystals based on (a) holes,<sup>33</sup> (b) corrugations,<sup>34</sup> (c) wings,<sup>35</sup> and (d) pillars.<sup>36</sup> The scale bar is 300 nm. (e) TEM image of a carbon nanotube with periodically encapsulated fullerene molecules.<sup>37</sup> Reproduced with permission from Kodama *et al.*, *Nat. Mater.* **16**, 892–897 (2017). Copyright 2017 Nature Publishing Group. (f) Reduction in the thermal conductivity of various nanostructures<sup>14,36–38</sup> caused by addition of various scatterers.

in disordered systems. Moreover, these effects were temperature-dependent and disappeared above 10 K, in agreement with models.<sup>33,69</sup>

Another type of nanostructure that could be considered 1D phononic crystals consists of periodic pillars placed on top of a nanobeam, as shown in Fig. 3(d). Simulations typically predict the thermal conductivity reduction due to the coherent phonon resonances in the pillars even at room temperature.<sup>7</sup> However, experiments could only show the thermal conductivity reduction [Fig. 3(f)] due to incoherent effects, specifically due to additional phonon scattering on the boundary between pillars and the beam.<sup>36</sup>

Thus, in the systems with characteristic dimensions of hundreds of nanometers, the main factor causing the reduction in thermal conductivity seems to be the incoherent surface scattering, especially at room temperature. Indeed, phonons are likely to lose their coherence over the distances of few hundred nanometers due to the phonon–phonon scattering processes at room temperature;<sup>71–73</sup> thus, even if coherent surface scattering events occur, they cannot cause phonon interference. For this reason, coherent effects are more likely to have a noticeable impact at low temperatures where the coherent surface scattering due to the longer phonon wavelength and the longer mean free path due to rarer phonon–phonon scattering make it possible to preserve coherence over hundreds of nanometers.<sup>71</sup>

However, in systems of smaller dimensions, the coherent effects might have a more significant impact even at room temperature. Kodama *et al.*<sup>37</sup> demonstrated a reduction in the thermal conductivity of carbon nanotubes due to periodically encapsulated fullerene molecules, as shown in Figs. 3(e) and 3(f). They attributed this reduction to the coherent modifications of phonon dispersion caused by the periodic strain induced by encapsulated molecules.

## COHERENT HEAT CONDUCTION IN SUPERLATTICES

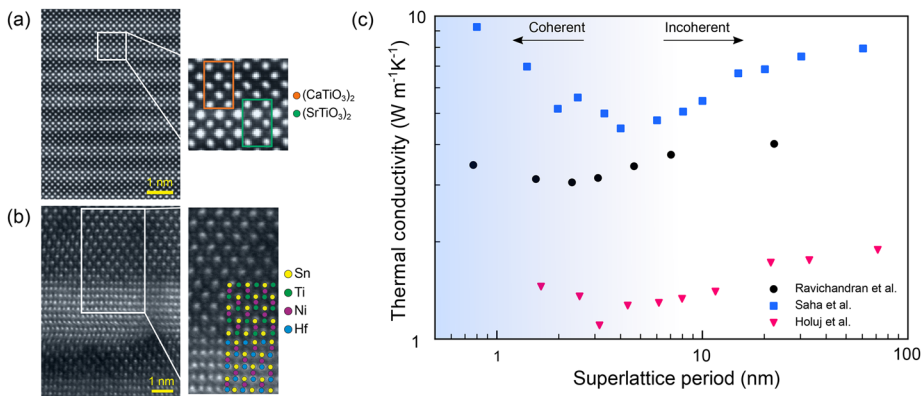
Superlattices are essentially the simplest 1D phononic crystals. The thermal conductivity of superlattices is usually lower than

that of bulk materials.<sup>74–76</sup> This reduction can be caused by both coherent and incoherent effects.<sup>64,72</sup> Indeed, due to the nanometer scale periodicity and atomically flat interfaces between the layers, phonon coherence in superlattices can be preserved over several layers, thus suppressing heat conduction coherently due to the periodicity of the layers.<sup>75,77</sup> On the other hand, the high density of the interfaces between the layers creates a medium where phonons tend to be scattered diffusely, thus suppressing heat conduction incoherently.<sup>78</sup>

The competition between coherent and incoherent effects is one of the central topics in the literature on superlattice heat conduction. Theoretical works predicted a gradual transition from incoherent to coherent heat conduction as the superlattice period becomes shorter.<sup>75,77</sup> In other words, in superlattices with long periods, phonons may not yet feel the periodicity of the layers and thus are mainly affected by the diffuse scattering at the layer interfaces.<sup>79</sup> As the period gets shorter, interfaces become denser, which only makes the diffuse scattering more frequent and the thermal conductivity lower. However, when periods become as short as several nanometers, the phonons start feeling the periodicity, and heat conduction becomes coherent, which inverses the decreasing trend in the thermal conductivity.

To demonstrate this transition experimentally, Ravichandran *et al.*<sup>64</sup> measured oxide superlattices. They showed how the thermal conductivity reaches a minimum at the periodicity of about 2 nm and starts increasing again as the period is reduced further (Fig. 4). Moreover, at lower temperatures, this crossover occurred at longer periods due to the longer wavelength and mean free path of phonons at lower temperatures. Later works<sup>65,66</sup> demonstrated a similar transition into the coherent regime in metal/semiconductor superlattices at longer periodicities of about 5 nm (Fig. 4), albeit without a clear dependence of the crossover point on the temperature.

Another effect prominent in superlattices is Anderson localization—the phenomenon of wave localization in disordered media. When disorder is large enough, the random scattering of propagating Bloch modes leads to a strong localization with a characteristic length scale much shorter than the length of the



**FIG. 4.** TEM images of (a)  $(\text{STO})_m/(\text{CTO})_n$  and (b)  $\text{TiNiSn}/\text{HfNiSn}$  superlattices.<sup>64,65</sup> (c) Thermal conductivity as a function of the superlattice period at 300 K reported in the literature.<sup>64–66</sup> The trends show the crossover from incoherent to coherent heat conduction. (a) Reproduced with permission from Ravichandran *et al.*, *Nat. Mater.* **13**, 168–172 (2014). Copyright 2014 Nature Publishing Group.

structure. Specifically, narrow resonances appear at the band edges and form bands of localized modes that broaden with increasing disorder. Theoretical works predict that thermal phonons can become localized in aperiodic superlattices, which leads to the suppression of phonon transport that can theoretically reduce the thermal conductivity by up to two orders of magnitude.<sup>72,80–82</sup> Experimentally, the evidence of such localization has been observed in GaAs/AlAs superlattices with randomly distributed islands of ErAs.<sup>83</sup> In addition, Anderson localization can enhance the optomechanical coupling.<sup>47,48</sup>

As far as the thermal conductivity reduction in superlattices is concerned, researchers even predicted the thermal conductivity below the amorphous limit.<sup>84–86</sup> These predictions were experimentally confirmed in various amorphous and crystalline superlattices.<sup>87–89</sup> However, this ultra-low thermal conductivity is mainly attributed to the incoherent phonon scattering.

## SUMMARY

We reviewed the last decade of advances in phonon and heat manipulations in 1D phononic structures. At the hypersonic frequencies, 1D phononic crystals became an important part of optomechanical devices, enabling a fine control over photonic and phononic properties. This leads to interesting effects, such as phonon lasing, cooling, and synchronization of mechanical cavities at the nanoscale. These functions stem from the possibility of strongly confining phonon modes in cavities surrounded by Bragg mirrors designed around specific frequencies. Current developments tend toward building networks of such OM nanobeams to create phonon circuits that work at well-defined frequencies or push limits of the sensors.

However, at terahertz frequencies, when collective phonon motions essentially results in heat, the possibility of using phonon interference is not yet clear. In wire-based 1D phononic crystals, most reports remain skeptical about the possibility of coherent heat conduction at room temperature. Theoretical works discuss this possibility either at ultra-low temperatures or in ultra-small structures with the characteristic size of several atomic lattices. Most experiments, however, measured nanostructures with periodic features of several tens of nanometers in size. The results suggest that these periodic features act merely as additional scattering points, making heat conduction even more diffusive than in pristine

nanowires and beams. Nevertheless, all the experimental works measured a substantial reduction in the thermal conductivity caused by the periodic features. Thus, 1D periodic structures can still suppress thermal transport in applications involving thermal isolation, albeit incoherently.

The situation seems more optimistic in atomically small systems. Experiments on carbon nanotubes with periodically encapsulated molecules or superlattices with periodicity below 5 nm detected a possible coherent suppression of the thermal conductivity even at room temperature. Thus, while coherent control over heat conduction seems possible in principle, the nanostructures capable of such control are yet to be developed.

Summarizing, while low-frequency 1D phononic crystals successfully found applications in optomechanics, high-frequency structures are still struggling to demonstrate their efficiency for heat manipulations. Future research should try to miniaturize phononic structures further and improve their surface quality. This should enable better preservation of the phonon phase over a larger number of periods and lead to a more substantial impact of phonon interference at higher temperatures.

## ACKNOWLEDGMENTS

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## DATA AVAILABILITY

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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