A coherent phonon pulse model for transient phonon thermal transport

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In this work, we present a novel heat source model, the *coherent phonon pulse* (CPP), composed of spatiotemporal Gaussian wave packets to mimic the coherent excitation of a non-equilibrium phonon population by ultrashort laser techniques, for the study of transient phonon thermal transport. Through molecular dynamic simulations of phonon transport in bicrystalline silicon-nanowires containing $\Sigma 3$ and $\Sigma 19$ grain-boundaries (GBs), we demonstrate that the new model facilitate not only a quantitative measurement of phonon-interface scattering, but also a mechanistic understanding of the highly non-equilibrium process of phonon transport with the coherent wave nature being preserved.

Keywords: Computational model, coherent phonons, ultrashort laser pulse, transient phonon transport

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1. Introduction

The advances in time-resolved experimental studies of thermal transport, especially in the study of transient non-equilibrium heat flow using pump-probe laser pulse methods, have led to discoveries of many new phenomena, and have produced a wealth of challenges for the simulation community to interpret the experiments [1]. In particular, the pump-probe technique has become a leading transient thermal metrology not only for the measurement of thermal conductivity and interfacial thermal conductance, but also for observation of coherent phonon transport [2]. Despite the rich pool of experimental studies, however, there is currently no well-established simulation method that can mimic either the coherent phonon generation or the process of the coherent phonon pulse propagation and scattering. A key component that is missing is a heat pulse model that can mimic the phonon population excited by laser pulses.

A laser pulse generates a local concentration of non-equilibrium phonons. According to Msaal and Wolfe [3], the generated non-equilibrium phonons highly depend on the “excitation density” (or absorbed laser power per area) and the properties of the sample material. Although the process of phonon generation and the resulting complex phonon oscillation are still a topic of study [4], using ultrashort laser techniques, several research groups have demonstrated that the propagation of the light pulses in solids is accompanied by lattice vibrations showing a high degree of spatial and temporal coherence [4-7]. Coherent phonon generations are observed from the Γ -point phonons to the near-Brillouin zone boundary phonons, including acoustic and optical phonons [8-10]. Such excitation and detection of coherent lattice vibrations has been observed in many transparent and opaque materials, such as transition

metals [11], semi-metals [12-17], cuprates [18], insulators [19] and semiconductors [20-22]. Several mechanisms were proposed to explain the coherent phonon generation [23,24]. A widely accepted view is that, when the duration of laser pulse is short enough, the phonons are excited coherently. Coherence is a general phenomenon that takes place whenever the ultrashort laser interacts with solid [25].

The atomic-level molecular dynamics (MD) simulation is a powerful tool that can be used to simulate transient non-equilibrium process without the need of a priori information of phonon properties. The most widely used non-equilibrium MD simulation method for the calculation of thermal conductivity or thermal conductance is the direct method, i.e., the heat source-sink method, which is in analogy to the experimental steady-state measurement [26-28]. To determine the thermal conductance (σ_k) of an interface, this method uses a thermal model, $\sigma_k = J / \Delta T$, where J is the steady state heat current and ΔT is the temperature discontinuity at the interface. However, this method cannot provide the fine details that reveal the underlying mechanisms about phonon-interface scattering, which is critically important in the study of nanoscale thermal transport.

In order to gain information about phonon scattering mechanism, the phonon wave-packet dynamics method (PWD) [29,30] has been developed [31], and shown to be instructive in the mechanistic study of an individual phonon with a specific polarization and wavevector. In addition, by calculating the energy transmission coefficient of each phonon, the theoretical thermal conductance can be obtained [27,32]. However, to predict the thermal boundary conductance, many simulations have to be performed to determine the energy-transmission coefficient for each

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polarization and each wavevector. The contribution of each phonon is then superimposed according to a theoretical model based on the thermodynamic equilibrium Bose distribution [27]. Currently this method is essentially a zero-temperature method, the anharmonicity or phonon-phonon interaction that may accompany the ballistic phonon transport processes is basically ignored [29].

The direct method is very useful for quantitative study of steady-state heat flow, while the wave packet method is the method of choice for the mechanistic study of the scattering of individual phonons by interfaces. Unfortunately, neither method is well suited for the simulation of the generation and propagation of a phonon pulse. Existing attempts to study the transient heat pulse propagation have used the thermostat algorithms to model the heat source [33-35]. However, thermostat algorithms mimic thermalizing events such as damping and dephasing of phonon waves. As a result, the phase information or the phonon coherency is usually completely or partially destroyed [36]. Therefore, they are also not well suited for the simulation of the coherent phonon excitation by ultrashort laser pulses.

Motivated by the need of a heat pulse model to mimic the coherent phonon excitation and inspired by the time-resolved experimental studies, in this paper we propose a heat source model called *coherent phonon pulse* (CPP) model to mimic the coherent phonon excitation in the ultrashort laser pulse experiments.

2. The CPP model

Coherence is the key property of the phonons excitations generated in solids by the ultra-short laser pulse. The spatial and temporal coherence of phonons can be mathematically represented by phonon wave packets [37]. In addition, experiments show that most of the incident pump laser pulses can be described in a Gaussian profile [23,38-40]. Also, a laser pulse generates a local concentration of nonequilibrium phonons, and the number of phonons excited can be linked to the local temperature associated with the heat pulse [41].

Based on the results of the experimental studies as well as considerations mentioned above, in this work, we construct the CPP model from spatiotemporal Gaussian phonon wave packets. The general mathematical description of such wave packets can be given as follows:

$$u_{i\mu\lambda}(r, t) = \sum_{j=1}^n A_j \varepsilon_{ji\mu\lambda} \exp[i(k_j(r - r_0) - \omega_j(t - t_0))] \exp[-\frac{(t - t_0)^2}{\xi_j^2}] \exp[-\frac{(r - r_0)^2}{\eta_j^2}] \quad (1)$$

where $u_{i\mu\lambda}(r, t)$ is the μ -th component of the displacement of atom i polarized along $\varepsilon_{ji\mu\lambda}$ in the designated unit cell located at position r ; the phonon branch is labelled by λ ;

r_0 and t_0 are the center of the wave packet in spatial and temporal domain, respectively. The summation over j accounts for the combination of n Gaussian waves, which form a specific phonon distribution; k_j , ω_j , η_j and ξ_j are central wavevectors, frequencies and variances of the Gaussian wave packets in spatial and temporal domain. The magnitude A_j of each wave packet can be determined through the temperature and the phonon distribution associated with the heat pulse. The applied transient atomic vibration according to Eq. (1) gives rise to a coherent heat source comprised of Gaussian wave packets in both spatial and temporal domain. Note that when 1D transport is considered without time dependence or a specific distribution, the CPP model reduces to the phonon wave-packet dynamics.

The salient features of the CPP model can be summarized as follows. It mimics the ultrashort laser pulse experiments generating an ensemble of phonons, enables the wave nature of phonon thermal transport to be retained, and allows for the transient characterization in thermal conduction regime where Fourier's Law breaks down. In experiment, the control of phonons has to be realized through a precise modulation of the light source [25], while using the CPP model with MD simulation we can directly assign the transient atomic motion. In addition, to characterize the material properties, we directly track the atomic trajectories everywhere in the specimen without the need of other assumptions. This also significantly simplifies the data analysis, which is complex in experiment [38]. At the simplest level, the effect of the grain boundary (GB) can be characterized in terms of phonon transmittance [30]. Thus, for any ensemble of phonons of interest, we calculate the corresponding energy-transmission coefficients of the interfaces. Moreover, the intrinsic scattering, i.e., the phonon-phonon interaction at finite temperature are naturally allowed using the CPP model.

3. Simulation results

We apply this model in molecular dynamics (MD) simulation to study the non-equilibrium transient phonon thermal transport in silicon nanowires (SiNWs) with grain boundaries (GBs). We choose SiNWs because of the coexistence of coherent and incoherent phonon transport during the process of heat transfer due to the intensive surface scattering. GBs are introduced in order to demonstrate the capability of this new model in studying the thermal boundary resistance (TBR) problem.

Since SiNW provides a quasi-1D channel for energy transport, Eq. (1) can be reduced to

$$u(z_0, t) = \sum_{j=1}^n A_j \varepsilon_{ji\mu\lambda} \exp[i\omega_j(t - t_0)] \exp[-\frac{(t - t_0)^2}{\xi_j^2}] \quad (2)$$

where $u(z_0, t)$ is the transient displacement of the 1st atom in the designated unit cell located at z_0 , at time t . All the

other symbols follow the definition in Eq. (1). In addition, we do not differentiate acoustic and optical phonons since they are no longer relevant in nanostructures due to the phonon dispersion modification [42]. Hence, the displacement of the 2nd atom is not controlled, but solved in the simulation according to the equation of motion. Since the phonon density of state (PDOS) is one way to link the phonon distribution to the temperature within the framework of classical mechanics, in this work, we construct the CPP according to the PDOS of the material.

The resulted displacement of the CPP is plotted in Fig. 1 (a). The corresponding frequency domain analysis by Fourier transform is presented in Fig. 1 (b), from which, the heat pulse can be identified as four Gaussian waves (the central frequency of the last two Gaussian waves are close). The inset in Fig. 1 (b) is the PDOS of single crystal SiNW at 500K, which is obtained by calculating the Fourier transform of the velocity-velocity autocorrelation from the trajectories of atoms in a MD simulation [43,44]. Comparing Fig. 1 (b) with the inset, we conclude that the heat pulse input we constructed is a rough representation of the PDOS.

Fig. 1: (a) Wave packet composed of Gaussian waves. (b) Fourier Transform of the wave packet in (a), inset in (b) is the PDOS of SiNW at 500K computed from MD results.

In Fig. 2, we present the schematic of the computational model ($\sim 600,000$ atoms, $\sim 3\text{nm} \times 3\text{nm} \times 1.2\mu\text{m}$). The general-purpose molecular dynamics software package LAMMPS [45] is employed in all the simulations in this work without assuming periodic boundary conditions. Velocity Verlet algorithm with time step of 0.55fs is used, which is about 1% of the shortest phonon period in Si lattice. Before the heat pulse is generated, the MD model is equilibrated at 0.1K to allow only the scattering events that involve phonons generated from the heat source. Note that with a higher initial temperature, the scattering events involve the original thermal phonons can be naturally incorporated. Thereafter, the heat pulse constructed by CPP model is applied in the middle of the Grain I, and naturally allowed in the MD simulations to propagate across the GBs into the Grain II (positive z) and the Grain III (negative z) at the two ends of the NW. With the heat source region located at the center of the Grain I, unwanted phonon scatterings by free boundaries are avoided. Since the model is symmetric, only half of which is of interest, we take it as a

“bicrystalline” model. The NW is divided into 1000 slabs along z direction; each slab is 12 Å, consisting of 600 atoms. The kinetic temperature of each slab T_{KEi} is statistically measured by averaging the kinetic energy over n atoms within the slab, and over a time period of t_{average} , which is chosen to be 500 time steps. The mathematical description is

$$T_{KEi} = \frac{1}{t_{\text{average}}} \sum_{\tau} \frac{1}{3nk_B} \sum_{k=1}^n m_k (v_k(\tau) - \bar{v}(\tau))^2 \quad (3)$$

where $\bar{v}(\tau) = \frac{1}{n} \sum_{k=1}^n v_k(\tau)$ and k_B is the Boltzmann constant.

Fig. 2: (Colour on-line) Schematic drawing of MD model of “bicrystalline” SiNW subjected to heat pulse.

Figure 3 presents the atomic structure of the GBs in the “bicrystalline” SiNW models obtained by MD simulation using Stillinger-Weber potential [46]. Fig. 2 (a) presents the $\Sigma 3$ coherent twin boundary along $\{111\}$ plane. The tilt angle between the two grains is 70.53° , and the GB energy is almost zero. Presented in Fig. 2 (b) is the $\Sigma 19$ GB along $\{133\}$ plane, the tilt angle is 26.53° , and the GB energy is 0.50 J/m^2 . The details of the GB energy calculation and the comparison between the GB atomic structures obtained by MD simulations and those obtained by Tight-binding calculations have been presented in a previous work [47].

Fig. 3: Atomic-structure of GBs in the “bicrystalline” SiNWs (a) $\{111\}$ $\Sigma 3$ GB and (b) $\{133\}$ $\Sigma 19$ GB.

Since in the CPP model the heat pulse is constructed from phonon wave packets, different combinations of the latter can be investigated. To isolate the contribution of the longitudinal and the transverse phonons to GB conductance, we conduct MD simulations using CPP models composed of the longitudinal and the transverse phonons, respectively. In the rest of this paper, we call them “CPP-Longitudinal” and “CPP-Transverse”. Both of them follow the same distribution shown in Fig. 1.

In Fig. 4 we present the spatiotemporal isotherm contours obtained from the MD simulations of heat conduction process in the three models, namely, the $\langle 111 \rangle$ oriented single crystal SiNW, the bicrystalline SiNW with $\Sigma 3$ GB, and the bicrystalline SiNW with $\Sigma 19$ GB, respectively. All the three models are subjected to CPP-Longitudinal and of CPP-Transverse. For comparison, we also perform MD simulations with the local heat pulse modeled by the Nosé-Hoover thermostat algorithms [33], and we call it “Thermostat-HP” in the rest of the paper. To compare with the Thermostat-HP, we control in CPP model the generated peak kinetic temperature through tuning the amplitudes in Eq. (2). Thus, in all the nine simulations presented in Fig. 4, the local temperature in the heated region is maintained as $T_{peak} = 500K$ for 1ps, and then the systems are time integrated for 250ps. Due to the symmetric computational setup, only one half of the contours are plotted.

Figure 4(a)-(c) present the isotherms of heat conduction in the three models subjected to CPP-Longitudinal. It is seen that the processes of the propagation of phonon waves, their interactions with GBs, and their reflections by the free surfaces are clearly discernible, indicating the wave natures of phonon thermal transport. In the single crystal SiNW model shown in Fig. 4(a), we observe some phonon waves propagate with constant group velocities without decaying. The sound velocity can be measured from the 1st wave front propagation (dashed line in Fig. 4(a)), which is about 7.5km/s. This value is in good agreement with a recent theoretical work [42] on $\langle 111 \rangle$ SiNW. On the contrary, in the bicrystal models shown in Fig. 4(b) and 4(c) we observe that the wave fronts are impeded by the GBs (the location of GBs are indicated by the black arrows), resulting in temperature discontinuities. Meanwhile, we note that the temperature discontinuity at the $\Sigma 19$ GB in Fig. 4(c) is much more significant than that at $\Sigma 3$ GB in Fig. 4(b), indicating that a much larger amount of longitudinal waves has been hindered by the $\Sigma 19$ GB.

Fig. 4: Spatiotemporal isotherms of single crystal SiNW, SiNW with $\Sigma 3$ GBs, and SiNW with $\Sigma 19$ GBs subjected to CPP-Longitudinal (a-c), to CPP-Transverse (d-f), and to Thermostat-HP (g-i). (The color bar indicates the amplitude of temperature in Kelvin)

Figure 4(d)-(f) present the isotherms of heat conduction in the three models subjected to CPP-Transverse. It is seen that as expected, the wavepackets constructed out of the transverse phonons propagate in a less wave-like behavior and with much lower group velocities. Similarly, the transverse sound velocity can also be estimated by calculating the group velocity of the 1st wave front (dashed line in Fig. 4d), which is around 4km/s; this value is also in good agreement with literature [42]. Comparing Fig. 4(e) and 4(f), we find that with CPP-Transverse, the difference between the temperature continuity at $\Sigma 3$ and that at $\Sigma 19$ is not as significant as that with CPP-Longitudinal shown in Fig. 4(b) and 4(c).

We present in Fig. 4(g)-(i) the isotherms of heat conduction in the three models subjected to Thermostat-HP. Again, in Fig. 4(h) and 4(i), we observe temperature discontinuity at the GBs, and the discontinuity at the $\Sigma 19$ GB in Fig. 4(i) is more significant than that at the $\Sigma 3$ GB in Fig. 4(h). However, no obvious wave nature of the thermal transport can be observed in the spatiotemporal isotherms in Fig. 4(g)-(i), nor can it be observed by investigating spatiotemporal isotherms calculated based on velocity components only along x, y or z direction. This phenomenon is not in good agreement with the heat pulse experiments. In experiment, it is shown that when the heat source region is smaller than the phonon mean free path, the energy-carrying phonons travel ballistically away from the source for a significant distance before experiencing collisions [48]. We believe that using the Thermostat-HP model, the continuous velocity rescaling algorithm applied

at the heat source region, although only for a very short time, has created extra damping and dephasing which has destroyed the phonon coherency. By contrast, it is seen from Fig. 4 that the CPP model is able to retain the wave nature of phonon transport, which enables the visualization of the quasi-ballistic non-equilibrium transient phonon propagation and scattering with interfaces.

Table 1: Energy-transmission coefficients of $\Sigma 3$ and $\Sigma 19$ GBs subjected to heat pulse with CPP-Longitudinal, CPP-Transverse and Thermostat-HP models, respectively.

	$\Sigma 3$	$\Sigma 19$
CPP-Longitudinal	0.88	0.55
CPP-Transverse	0.80	0.77
Thermostat-HP	0.84	0.56

With the CPP model, we can also calculate the energy transmission coefficients of the GBs. By recording the kinetic energy of the atoms in the Grain I and the Grain II at the end of each simulation, the transmitted energy in bicrystal models can be defined as the fraction of the incident energy in the Grain I that propagates across GB into the Grain II. For comparison, we also divide the single crystal model into the “equivalent Grain I” and the “equivalent Grain II” by the location of GBs in bicrystal models, and calculate the “equivalent transmitted energy”. Then the energy-transmission coefficients are defined as the ratio between the transmitted energy in bicrystal model and the “equivalent transmitted energy” in single crystal model. The results are summarized in Table 1. First, it is clear that the transmission coefficient of the $\Sigma 3$ GB is always larger than that of the $\Sigma 19$ GB. This suggest that introducing an effective GB such as $\Sigma 19$ GB can further reduce the thermal conductivity of SiNWs for a thermoelectric application. Second, it is seen that the transmission coefficients calculated from the Thermostat-HP model are always in between the coefficients calculated from the CPP-Longitudinal model and the CPP-Transverse model, as listed in Table 1. This implies that the measured overall thermal boundary resistance of each GB by the two models are quantitative close. Third, the transmission coefficients of the $\Sigma 3$ GB measured from the MD simulation with Thermostat-HP model is 0.84, and are respectively 0.88 and 0.80 with the CPP-Longitudinal and the CPP-Transverse model. These values show that the $\Sigma 3$ twin GB has a relatively high thermal conductance and scatters the longitudinal phonons only slightly stronger than the transverse phonons. However, for $\Sigma 19$ GB, the transmission coefficients calculated is 0.56 with the Thermostat-HP model, while are 0.77 and 0.55 with the CPP-Longitudinal and the CPP-Transverse model, respectively. This indicates that the $\Sigma 19$ GB has a much lower overall thermal conductance which is mainly resulted from the low transmission of longitudinal phonons.

These results presented in Table 1 are consistent with the contours presented in Fig. 4. Both of them demonstrate that $\Sigma 19$ GB is a much stronger thermal barrier than $\Sigma 3$ GB, and the strong thermal barrier mainly results from hindering the propagation of longitudinal phonons. The simulation results also indicate that with all possible phonons being considered, the CPP model can be used to quantify the overall thermal conductance as the Thermostat-HP model does. In addition to that, the CPP model can be used to differentiate contributions of different phonon ensembles, which is not attainable by using a Thermostat-HP model.

4. Conclusions

We have proposed a new heat source model, the CPP (coherent phonon pulse) model, and have demonstrated through MD simulation of bicrystalline SiNWs that this new model can be used to both quantify and understand the TBR (thermal boundary resistance) in ballistic-diffusive transition heat conduction regime. Simulation results of this work show that the CPP model naturally retains the wave nature of ultrafast heat pulse, reproduces the spatial and temporal coherences of phonons, and enables the visualization of the propagation of highly non-equilibrium phonons generated by the ultrashort laser pulse as well as the scattering of phonons by grain boundaries, thus proving information for a mechanistic understanding of phonon-interface scattering. In addition, this atomic vibration-based, Gaussian wave packets formed heat pulse with specific phonon modes enables the investigation of phonon ensembles of interest. By differentiating the contributions between the longitudinal and transverse phonons, we find that the TBR of the two GBs studied in this work exhibit only a small discrepancy for transverse phonons, however, differ significantly for longitudinal phonons, which result in the distinct overall TBRs. Also, the simulation results show that by considering all possible phonons, the overall thermal conductance obtained by using the CPP model are comparable with that by the thermostat induced heat-pulse model. This result implies that the quantitative value of the grain boundary thermal conductance does not highly depend on the heat pulse model.

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- [1] R.B. Wilson, J.P. Feser, G.T. Hohensee, D.G. Cahill, *Physical Review B* 88 (2013) 144305.
- [2] D.H. Hurley, S.L. Shinde, V.E. Gusev, *Journal of the Korean Physical Society* 57 (2010) 384.
- [3] M.E. Msall, J.P. Wolfe, *Phys. Rev. B* 65 (2002) 195205.
- [4] Y. Wang, L. Guo, X. Xu, J. Pierce, R. Venkatasubramanian, *Physical Review B* 88 (2013) 064307.
- [5] A. Huynh, B. Perrin, B. Jusserand, A. Lemaître, *Applied Physics Letters* 99 (2011).
- [6] K. Mizoguchi, M. Hase, S. Nakashima, M. Nakayama, *Physical Review B* 60 (1999) 8262.
- [7] R. Merlin, *Solid State Communications* 102 (1997) 207.
- [8] K. Mizoguchi, H. Takeuchi, T. Hino, M. Nakayama, *Journal of Physics: Condensed Matter* 14 (2002) L103.
- [9] H. Takeuchi, K. Mizoguchi, T. Hino, M. Nakayama, *Physica B: Condensed Matter* 316–317 (2002) 308.
- [10] I. Katayama, K. Sato, S. Koga, J. Takeda, S. Hishita, H. Fukidome, M. Suemitsu, M. Kitajima, *Physical Review B* 88 (2013) 245406.
- [11] M. Hase, M. Kitajima, S.-i. Nakashima, K. Mizoguchi, *Physical Review Letters* 88 (2002) 067401.
- [12] T.K. Cheng, S.D. Brorson, A.S. Kazeroonian, J.S. Moodera, G. Dresselhaus, M.S. Dresselhaus, E.P. Ippen, *Applied Physics Letters* 57 (1990) 1004.
- [13] H.J. Zeiger, J. Vidal, T.K. Cheng, E.P. Ippen, G. Dresselhaus, M.S. Dresselhaus, *Physical Review B* 45 (1992) 768.
- [14] K. Sokolowski-Tinten, C. Blome, J. Blums, A. Cavalleri, C. Dietrich, A. Tarasevitch, I. Uschmann, E. Forster, M. Kammler, M. Horn-von-Hoegen, D. von der Linde, *Nature* 422 (2003) 287.
- [15] G.A. Garrett, T.F. Albrecht, J.F. Whitaker, R. Merlin, *Physical Review Letters* 77 (1996) 3661.
- [16] M. Hase, K. Mizoguchi, H. Harima, S. Nakashima, M. Tani, K. Sakai, M. Hangyo, *Applied Physics Letters* 69 (1996) 2474.
- [17] S.L. Johnson, P. Beaud, C.J. Milne, F.S. Krasniqi, E.S. Zijlstra, M.E. Garcia, M. Kaiser, D. Grolimund, R. Abela, G. Ingold, *Physical Review Letters* 100 (2008) 155501.
- [18] W. Albrecht, T. Kruse, H. Kurz, *Physical Review Letters* 69 (1992) 1451.
- [19] K. Ishioka, M. Kitajima, O.V. Misochko, *Journal of Applied Physics* 100 (2006) 093501.
- [20] A. Rousse, C. Rischel, S. Fourmaux, I. Uschmann, S. Sebban, G. Grillon, P. Balcou, E. Forster, J.P. Geindre, P. Audebert, J.C. Gauthier, D. Hulin, *Nature* 410 (2001) 65.
- [21] M.N. Luckyanova, J. Garg, K. Esfarjani, A. Jandl, M.T. Bulsara, A.J. Schmidt, A.J. Minnich, S. Chen, M.S. Dresselhaus, Z. Ren, E.A. Fitzgerald, G. Chen, *Science* 338 (2012) 936.
- [22] J. Ravichandran, A.K. Yadav, R. Cheaito, P.B. Rossen, A. Soukiasian, S.J. Suresha, J.C. Duda, B.M. Foley, C.-H. Lee, Y. Zhu, A.W. Lichtenberger, J.E. Moore, D.A. Muller, D.G. Schlom, P.E. Hopkins, A. Majumdar, R. Ramesh, M.A. Zurbuchen, *Nat Mater* 13 (2014) 168.
- [23] T. Garl, Doctor of Philosophy, Ecole Polytechnique, France, 2008.
- [24] P. Ruello, V.E. Gusev, *Ultrasonics* 56 (2015) 21.
- [25] M. Hase, M. Kitajima, *Journal of Physics: Condensed Matter* 22 (2010) 073201.
- [26] P.K. Schelling, S.R. Phillpot, P. Keblinski, *Journal of Applied Physics* 95 (2004) 6082.
- [27] S. Aubry, C.J. Kimmer, A. Skye, P.K. Schelling, *Physical Review B* 78 (2008) 064112.
- [28] A. Maiti, G.D. Mahan, S.T. Pantelides, *Solid State Communications* 102 (1997) 517.
- [29] P.K. Schelling, S.R. Phillpot, P. Keblinski, *Applied Physics Letters* 80 (2002) 2484.
- [30] D.G. Cahill, P.V. Braun, G. Chen, D.R. Clarke, S. Fan, K.E. Goodson, P. Keblinski, W.P. King, G.D. Mahan, A. Majumdar, H.J. Maris, S.R. Phillpot, E. Pop, L. Shi, *Applied Physics Reviews* 1 (2014).
- [31] B. Becker, P.K. Schelling, S.R. Phillpot, *Journal of Applied Physics* 99 (2006).
- [32] Z. Zheng, X. Chen, B. Deng, A. Chernatynskiy, S. Yang, L. Xiong, Y. Chen, *Journal of Applied Physics* 116 (2014).
- [33] J. Shiomi, S. Maruyama, *Physical Review B* 73 (2006) 205420.
- [34] S. Volz, J.-B. Saulnier, M. Lallemand, B. Perrin, P. Depondt, M. Mareschal, *Physical Review B* 54 (1996) 340.
- [35] T. Zolotoukhina, *Japanese Journal of Applied Physics* 49 (2010) 085001.
- [36] K. Sääskilähti, J. Oksanen, J. Tulkki, *Physical Review E* 88 (2013) 012128.
- [37] B. Latour, S. Volz, Y. Chalopin, *Physical Review B* 90 (2014) 014307.
- [38] D.G. Cahill, *Review of Scientific Instruments* 75 (2004) 5119.
- [39] M.V. Iravani, M. Nikoonahad, *Journal of Applied Physics* 62 (1987) 4065.
- [40] D.S. Ivanov, L.V. Zhigilei, *Physical Review B* 68 (2003) 064114.
- [41] C. Kittel, *Introduction to solid state physics*, Wiley, New York, 1966.
- [42] H. Karamitaheri, N. Neophytou, M. Taheri, R. Faez, H. Kosina, *Journal of Elec Materi* 42 (2013) 2091.
- [43] M.T. Dove, *Introduction to Lattice Dynamics*. Cambridge University Press, Cambridge, 1993.

- 1
2
3
4 [44] J.R. Lukes, H. Zhong, Journal of Heat Transfer 129 (2006) 705.
5
6 [45] S. Plimpton, Journal of Computational Physics 117 (1995) 1.
7
8 [46] F.H. Stillinger, T.A. Weber, Physical Review B 31 (1985) 5262.
9
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47
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51
52
53
54
55
56
57
58
59
60
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62
63
64
65
- [47] X. Chen, L. Xiong, A. Chernatynskiy, Y. Chen, Journal of Applied Physics 116 (2014) 244309.
[48] M.E. Siemens, Q. Li, R. Yang, K.A. Nelson, E.H. Anderson, M.M. Murnane, H.C. Kapteyn, Nat Mater 9 (2010) 26.