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A quasi-continuum thermomechanical model for phonon damping analysis of single crystal silicon nano-resonators

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ABSTRACT

In this paper, we study phonon-mediated intrinsic damping in single crystal silicon nano-resonators where the phonon transport is of partial ballistic and partial diffusive nature. For this purpose, we present a quasi-continuum thermomechanical model that accounts for both thermoelastic and Akhiezer energy dissipation mechanisms. In the model, the linearized frequency-dependent phonon Boltzmann transport equation (BTE) is coupled with continuum elasticity equations via phonon modulation theory. The model is implemented numerically by using the finite element and finite volume methods for calculating the damping ratio and quality factor of nano-resonators under forced vibration. Both flexural and axial motions are considered for single crystal silicon nano-resonators with different sizes and frequencies. The numerical results obtained from the quasi-continuum thermomechanical model are compared with those obtained from molecular dynamics simulations.

1. Introduction

The quality factor of nano-resonators, which is characterized by the ratio of energy stored to energy loss over a period of operation time, plays an important role in the performance and stability of nano-electromechanical devices [1]. In general, energy dissipation in nano-resonators can be categorized into two types: extrinsic dissipation and intrinsic dissipation. Extrinsic dissipation includes damping caused by the surrounding environment [2], material impurities [3], and structural support [4]. This type of energy dissipation can be reduced or even eliminated through optimized engineering design and manufacturing process. On the other hand, intrinsic dissipation is due to the system's inherent properties. For mechanical resonators, intrinsic dissipation mainly includes thermoelastic damping (TED) [5], Akhiezer damping [6] and surface damping [7]. TED occurs when a structural motion induced inhomogeneous strain field results in internal spatial heat flow, and hence thermal energy dissipation. TED is relatively well understood for micro-resonators. The classical TED theory [5,8,9] predicts a single-peak Lorentian behavior of the thermoelastic damping ratio in the frequency domain. Khisaeva and Ostoja-Starzewski [10] proposed a TED theory with second sound effects by adding the derivatives of heat flux into Fourier's law, which captures non-diffusive heat flow effects. Solutions of the modified theory show that the thermoelastic damping ratio contains many other peaks over the frequency domain [10,11]. While these models have been successfully applied to micro-resonators, they are not directly applicable to nano-resonators due to the fact that the heat flow in nanoscale structures is partially diffusive and partially ballistic in nature. In addition to TED, Akhiezer damping takes place due to the frequency-dependent phonon modulation caused by the same strain field and, consequently, the internal heat flow between the perturbed phonon groups of different frequencies. Such non-spatial but phonon-frequency-related heat redistribution leads to further energy dissipation. Akhiezer damping has received much attention in studies of nano-resonators, and has been compared with TED in terms of their relative importance. A number of research works including theoretical analysis [6,12], experiments [13], and molecular dynamics (MD) simulations [14] have concluded that the role of Akhiezer damping becomes significant when the resonator size becomes smaller than the phonon mean free path.

The thermal transport and dissipation mechanisms become different when the size of spatial domain reduces to nanoscale and the frequency of vibration reaches gigahertz level. For thermal transport, both Fourier's law and its modification with second sound effect have been shown to be inadequate in the nano-regime [15]. Instead, the phonon Boltzmann transport equation (BTE) model has been applied to thermal transport analysis in various nano-scale applications with demonstrated accuracy and efficiency [16–18], mainly because it views heat conduction as

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collective interactions of phonons and captures both diffusive and ballistic behavior of phonon transport through various scattering mechanisms. The BTE treatment in nano-scale thermal transport suggests that the intrinsic damping can be theorized in the light of phonon-mediated energy dissipation, in which the coupling between strain and phonons redefines the phonon distribution, transport and relaxation, and hence energy dissipation. With the BTE treatment in damping analysis, it is important to acknowledge that phonon distribution and transportation are spatial and frequency dependent. By incorporating the spatial dependence in the BTE model, one evaluates the coupling between the spatially inhomogeneous elastic and phonon fields, hence the nano-scale equivalence of TED. On the other hand, by incorporating the frequency dispersion in the BTE model, one evaluates the strain-induced local relaxation between phonon branches/modes, hence the Akhiezer damping. Altogether, the phonons are modulated, both spatially and between dispersion branches, by the strain field through the generalized frequency dependent Grüneisen tensor. The fundamental assumption is that the coupling between elastic strain field and phonon distribution can be established through the phonon modulation theory [6,19]. Several authors [20–22] have calculated the mode-dependent Grüneisen parameters that represent the strength of influence. In the light of this, Kiselev and Iafrate [23] developed a semi-analytical phonon-modulation damping model for flexural nano-beams and provided a qualitative view of the damping behavior as a function of beam length, aspect ratio and vibration frequency. However, the semi-analytical model is based on significant theoretical simplifications such as 1-D Euler–Bernoulli beam theory, the Debye model for phonon spectrum and 1-D thermal transport assumption. In addition, the strength of strain-phonon interaction is represented by only two distinctive Grüneisen parameters for the entire phonon dispersion. Kunal and Aluru [14] have recently investigated the Akhiezer damping of nano-bars using MD simulations and provided a clearer view of its relative importance as compared to surface damping. However, the atomistic simulation methods such as MD are cumbersome for damping analysis of nano-resonators due to the high computational cost in tracing time history of the dynamic response.

The above issues lead to the motivation of formulating the holistic damping mechanism, via the phonon modulation theory, into a coupled thermomechanical computational model for numerical analysis of intrinsic damping in crystalline nano-structures. In this paper, we present a quasi-continuum thermomechanical model for this purpose. It should be noted that, while the proposed model is applied to the intrinsic damping analysis of single crystal silicon nano-resonators in this paper, it is a general model and applicable to other crystalline materials. In the general framework of the model, lattice dynamics is adopted to calculate thermodynamic properties of the crystalline material such as phonon dispersion, mode-dependent Grüneisen parameters and elastic constants. With these properties as parameters, the phonon transport is described by frequency-dependent BTE to account for details of the phonon dispersion and phonon–phonon scatterings. This provides the treatment of the phonon redistribution in the Akhiezer damping. The strain field in the nano-structure is calculated by using the continuum elasticity theory considering thermal transport induced stress corrections. Furthermore, elastic scattering and structural boundary scattering of phonons are included in the BTE model. In short, the phonon BTE model is coupled with the continuum elasticity model through strain-induced phonon modulation and phonon transport induced stress corrections. The coupled thermomechanical model is solved numerically to obtain the damping ratio of nano-resonators. The finite element method (FEM) is employed for the discretization of the mechanical equation of motion. The finite volume method (FVM) is used for the discretization of the phonon BTE. Both flexural and axial motions are considered for nano-resonators with different lengths and frequencies. The numerical results obtained from the quasi-continuum thermomechanical model are compared with those obtained from MD simulations.

The rest of the paper is organized as follows. Section 2 illustrates the theoretical framework of the phonon-mediated damping theory. In Section 3, the numerical schemes and solution methods are described in details. Numerical results are presented in Section 4. Finally, Section 5 gives the conclusions.

2. Theory

Fig. 1 illustrates the theoretical framework of the quasi-continuum thermomechanical model. For single crystal Si, atomic interactions are described by using the Tersoff interatomic potential [24]. We then employ the lattice dynamics theory to compute thermodynamic and mechanical properties of the crystal lattice, including the phonon dispersion, mode-dependent Grüneisen parameters, phonon group velocity, specific heat, elastic constants, etc. These properties are incorporated into the frequency-dependent multi-band BTE for phonon transport analysis and the continuum elasticity theory for mechanical analysis. The phonon BTE is coupled with the continuum elasticity equations: the mechanical strain induces phonon modulation and phonon transport leads to mechanical stress corrections. The coupled equations are solved numerically and the damping ratio is calculated once the solution is obtained.

2.1. Thermodynamic properties of crystals

At the atomistic level, the interaction between atoms in the crystal lattices can be described by empirical interatomic potentials such as the Tersoff [24], Brenner [25] and Stillinger–Weber [26] potentials. Tersoff empirical interatomic potential is employed in this work for Si. Typically, the total potential energy U of a N-atom system is given by,

$$U = \sum_{\alpha} U_{\alpha} = \frac{1}{2} \sum_{\alpha \neq \beta} V_{\alpha\beta} \tag{1}$$

where α and β are the atoms of the system and $V_{\alpha\beta}$ is the bond energy between atoms α and β. For a crystal lattice under deformation, the phonon dispersion can be obtained by computing the

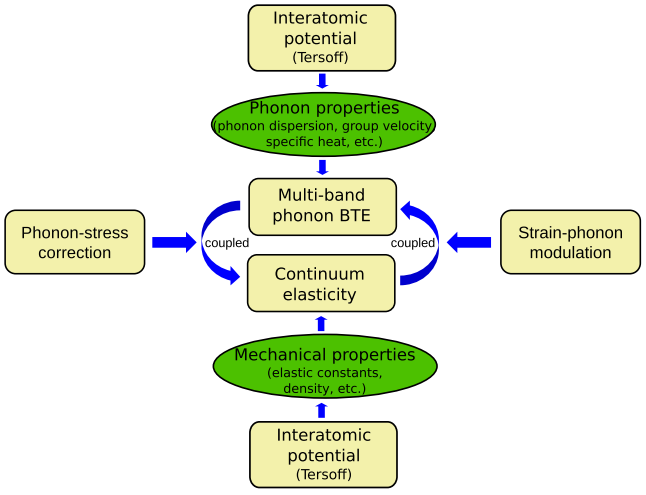

Fig. 1. The theoretical framework of the quasi-continuum thermomechanical model.

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