Computational Materials Science 110 (2015) 345–352

Contents lists available at ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

An efficient Laplace transform-wave packet method hybrid with substructure technique

Yunfeng Gu *

College of Electronic and Mechanical Engineering, Nanjing Forestry University, Nanjing 210037, PR China

ARTICLE INFO

Article history:
Received 18 February 2015
Received in revised form 26 August 2015
Accepted 27 August 2015

Keywords:
Wave packet method
Substructure
Inter-belt model
Laplace transform
Phonon transport

ABSTRACT

By virtue of substructure technique, the wave packet method can be applied to efficiently evaluate the thermal conduction of each phonon mode in the large periodic harmonic lattice. The substructures are connected by the inter-belts due to the long-range interatomic interaction. A parallel dynamic substructure method is presented in the Laplace transform domain, without any approximation in the condensation process. The validity and efficiency of the proposed method is demonstrated by the one- and three-dimensional cases. By launching a wide band wave packet, the whole given phonon branch can be studied by a one-time calculation. Defined as the ratio between square of Fourier transform of the transmitted and incident wave packets, the resulted transmission coefficient agrees with that obtained by the atomistic Green's function method. Moreover the time evolution of the wave field can be given by the method, and the multilevel substructure technique can also be used.

1. Introduction

The wave packet (WP) method [1–10] (or the phonon dynamics simulation [11]) is one of the most popular numerical methods used to study the phonon heat transfer mechanism at nanoscale [12]. Many factors affecting the phonon thermal transport can be easily taken into account, such as the anisotropy or phonon focusing [1], the phonon scattering at the defects [2], cavities [9], interface [3,4,7], edges [10] and the grain boundaries [6]. By this method, the phonon behavior in complex structures (e.g., the atomic-scale metamaterials [5], and the pillared graphene structure [8]) can also be simulated directly. The WP method is based on the molecular dynamics (MD) method [13], with a WP launched as the initial condition. Because the WP can have a narrow frequency range and well defined phonon polarization, the WP method is good at revealing the thermal transport mechanism of each phonon mode [6,11], and can play as a complementary approach to the MD method or the atomistic Green's function (AGF) method, which lumps together all the vibrations [14].

As a direct time integration method [13], the application of WP method is limited due to the high computational cost to solve large number of differential equations for a set of interacting atoms. The force evaluation according to the interatomic potential in every time step is also time consuming [13]. Although the anharmonic effects can be naturally included [1,5], the WP method is more likely to be a zero temperature method with the harmonic approximation [2,6,10]. Under the harmonic approximation, the thermal transport properties can be well explained [15], as long as the phonon mean free path (MFP) is longer than the characteristic length of the nanostructure. Furthermore, if the harmonic approximation is used, the time cost can be reduced by at least one order of magnitude [10].

One reason for the high computational cost is that large MD systems are required to localize the WP [16]. Periodic boundary conditions (PBC) are frequently used to acquire a finite simulation domain standing for an infinite one. However, in order to rule out the possible finite size effect [17], and to localize the WP, a sufficiently large system [3,7] must be taken even with the PBC. Sometimes the PBC will cause trouble. For example, in the simulation of the phonon focusing behavior [1], the WP signal is cluttered with the wave fronts that travel out of one boundary and wrap around to the opposing one. Without PBC, the WP propagation along the low-symmetry direction in graphene has been simulated in Ref. [10], in which the simulation system contains about 200,000–1,000,000 atoms with a time step of 0.1 fs.

To shorten the simulation time, the domain decomposition paradigm is used by Sun and co-workers [3]. In this paradigm, the entire domain is divided into several subsystems, and the calculation work of each subsystem is assigned to a particular

* Address: College of Electronic and Mechanical Engineering, Nanjing Forestry University, No. 159 Longpan Road, Nanjing, Jiangsu Province 210037, PR China.
E-mail address: gu_yunfeng@sina.com

http://dx.doi.org/10.1016/j.commatsci.2015.08.052
0927-0256/

processor. However, the total amount of calculation work has not been reduced yet.

To further reduce the computational cost, one has to explore a more efficient method. For example, as a domain decomposition algorithm in the finite element (FE) method, the substructure (SS) technique [18] has the ability to reduce the computing burden. Firstly, a large system is divided into several smaller subsystems, i.e., substructures (SSs). Then, the degrees of freedom (DOFs) of the internal nodes in the SSs are eliminated. As a result, the total system has only a greatly reduced number of DOFs belonging to the SS boundary nodes, and the computation cost is significantly lowered. The SS technique can also be applied to the atomic lattice, which is called the inter-belt (IB) model [19], because the SSs are connected by the IB form region due to the long-range interaction between atoms.

In this paper, the IB model is extended to the WP method for the harmonic atomic lattice. With the help of Laplace transform, the static condensation of DOFs is used without introducing the approximation [18]. For the harmonic atomic lattice, multiple WPs can be launched without coupled with each other nonlinearly [20]. By launching a broad band wave packet, the phonon transport behavior of a given branch can be studied more efficiently.

While MD is good at exploring anharmonic effects at high temperature, the proposed method herein focuses on coherent phonon transport at near zero temperature in a large structure. The harmonic force constants derived from the interatomic potential are used to form the stiffness matrix. The coherent heat effect is the key in nanoscale phononic crystal [21]. For the elastic wave propagation in the macroscopic phononic crystal, the research can rely on the finite difference time domain (FDTD) method and FE method [22]. A similar method can also be utilized for the nanoscale systems [23], but must be based on atomistic description. However, one prominent issue in the atomistic description is that there are too many atoms in the structure. For example, there are several hundreds of millions of atoms in silicon crystal with a size larger than the phonon mean free path [17]. The MD method can simulate an infinite system with one period by using the PBC. However, the period must be large enough to localize the WP, which will limit its application. Therefore, the simulation domain in many pervious studies is simplified into a nanowire shape, which is quasi one-dimensional [3,6,7]. The incident angles must be close to normal to the interface in the study of phonon thermal boundary resistance [24]. The SS technique can not deal with an infinite system, but can transform a large enough simulation domain into many SSs with a relatively cheap cost. Because there are only a few number of atoms remained in the IBs of the SS, the size of the resulted stiffness matrix is small. The SS technique is computationally efficient for the structure containing many repetitions of the same form [18]. Therefore, the modified WP method in this paper is especially suitable to handle the large periodic atomic structures. Once the SS stiffness matrixes have been prepared, the computational cost mainly depends on the size and the number of SS stiffness matrixes assembled into the global stiffness matrix of the structure.

This paper is organized as follows. In Section 2, the basic concepts of the method are described. The steps of the algorithm are detailed in Section 3. In Section 4, the atomic chains are taken as the toy examples to show the applicability of the method, and

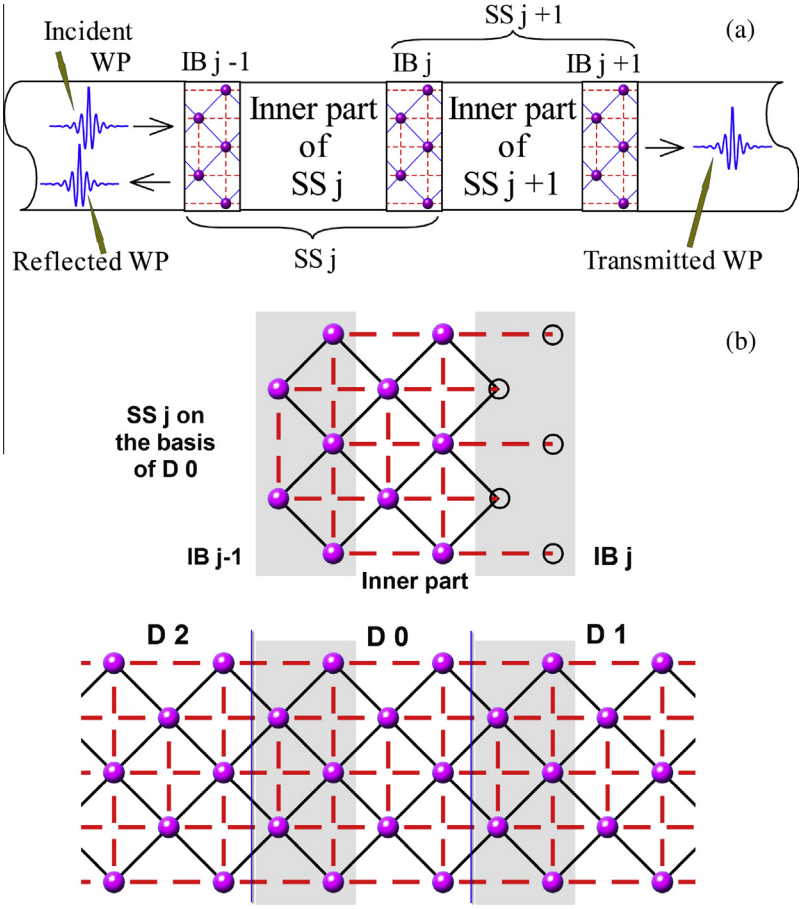

Fig. 1. (a) A schematic illustration of a structure divided into several substructures (SSs) connected with inter-belts (IBs) and (b) an example of substructure, SS *j*. There are three parts in SS *j*: the inner part, IB $j-1$ and IB *j*. The IBs have a grey background. The degrees of freedom (DOFs) of atoms in the inner part will be eliminated. A wave packet (WP) is launched and its transport process is observed by the IB atoms.