

Thermal conductivity of 1D carbyne chains



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ABSTRACT

Carbyne is a one-dimensional monoatomic chain of carbon atoms, consisting of repeating sp -hybridized groups – the extreme minimalist molecular rod or chain. Due to their potential use in atomic-scale circuits, there has been particular interest in their novel electronic and thermal properties and are promising platforms for heat dissipation. Potential 1D thermal transport is advantageous as the heat conduction can theoretically be directed along the molecule. However, the thermal properties of carbyne, essential to their successful application in the design of novel devices, have yet to be rigorously determined. Here, using full atomistic molecular dynamics (MD), we explore the thermal conductivity (κ) of a system of carbyne chains to enable statistical averaging. Müller-Plathe reverse perturbation method was used to obtain κ along the chain direction. For a freestanding chain with a length of approximately 40 nm, we indicate an ultrahigh thermal conductivity of approximately 0.793 kW/m-K, on the similar order of carbon nanotubes and graphene. Also, when we look into the thermal conductivity by atomistic weight, the carbyne model we use obtains a higher value than (5, 5) CNT and is comparable to graphene nanoribbon, which indicates very promising thermal conduction. Moreover, chains of varying length and strain are simulated individually to systematically explore the accessible range of conductivities. The thermal conductivity decreases when more strain applied, while it is significantly enhanced when we add more atoms to the carbyne chains. Additionally, we reported a close-to-linear relationship between κ and chain length, which provided supportive evidence for the controlling of thermal conductivity of carbyne.

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1. Introduction

Carbon allotropes have been a focus of research in last decades because of their molecular stability and exemplary properties, including thermal transport. Recently, a stable form of single carbon chain, carbyne, has been gaining attention as a promising carbon structure. It is a one-dimensional monoatomic chain of carbon atoms, consisting of repeating sp -hybridized groups – the extreme minimalist molecular rod or chain [1]. Theoretically, it may take a cumulene ($[=C=]$) repeating double bond form, or a polyene form with alternating single and triple bonds, which has been determined to be favorable because of its preferable energy status [2]; see Fig. 1. Carbyne has practical applications such as energy storage devices and nanoscale electronic devices. Most importantly, recent reports of successful synthesis of long chains of conjugated carbon provide a possibility for controlled production of carbyne in the polyene state [3]. Due to their potential use in atomic-scale circuits, there has been particular interest in

their novel electronic and thermal properties. Carbyne's larger 1D cousins – carbon nanotubes – have extremely high thermal conductivities (on the order of 6000 W/m-K [4,5]) and are promising platforms for heat dissipation in nanodevices.

In practice, the unavoidable presence of defects and interfaces results in a loss of the thermal transfer properties of CNT, as well as other materials, making predictive and reliable design difficult. Added to the fact that extreme heat gradients may facilitate defect formation, it is difficult to assume a constant value for the thermal conductivity of CNTs and other related nanoscale materials. In contrast, by definition, there can be no defects in a carbyne chain – introduction of such would effectively break the chain, and atomistic contact is lost. Simply put, it can be thought that defects introduce obstacles that heat transfer must traverse around, and thus any obstacle decreases thermal conductivity (indeed, the phonon paths are altered). The 1D nature of carbyne, however, only allows a single direction of heat transfer – as long as the chain is continuous, thermal conductivity cannot be impeded by “defects”.

Moreover, decrease in size to a single atomistic chain is promising, enabling the potential extraction of heat from junctions on the order of a few atoms, on the scale of Angstroms. Combined with

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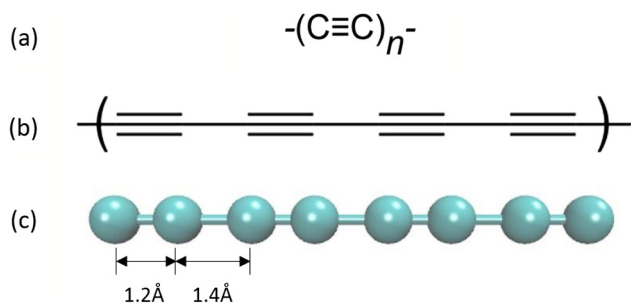


Fig. 1. (a and b) Formula and chemical schematic of *carbyne*, depicting the energetically favorable *polyyne* form with alternating single/triple carbon-carbon bonds. (c) Snapshot of part of model chain structure displayed in Visual Molecular Dynamic (VMD).

the unidirectional heat flux, carbyne chains may be able to efficiently transfer heat in extremely confined environments, without dissipating energy in transverse directions. Potential 1D thermal transport is clearly advantageous as the heat conduction can theoretically be efficiently directed along a desired direction. However, the thermal properties of carbyne, essential to their successful application in the design of novel devices, have yet to be rigorously determined. That being said, a recent study by Wang and Lin have used atomistic approaches to predict extremely high ballistic thermal transport in carbyne, dominated by axial acoustic modes [6]. At the same time, carbyne chains are highly flexible [2], suggesting significant bending motions. This poses fundamental questions about the connection of thermal properties and structure of carbyne and motivates us to explore more about it.

Many prior studies have been carried out using molecular dynamics to explore thermal transport mechanisms in low dimensional carbon materials. For example, Maruyama reported that the thermal conductivity of small diameter nanotubes represented no converging with the increase of length of nanotube while it obeys a striking power law relation [7]; Gang Wu illustrated that κ of finite length carbon chain is very high at room temperature and had a dependence on the chain size logarithmically [8]; meanwhile, Ge Yong found that external potentials could play an efficient role in improving the thermal conductivity of 1D carbon material [9]. The aforementioned study by Wang and Lin used nonreactive equilibrium modeling of a single carbyne chain to deduce conductivity [6]. Due to their monoatomic nature, complete understanding of the thermal properties of carbyne poses several challenges, including thermal distributions and sampling. Here, using full atomistic molecular dynamics (MD) with a reactive potential, we explore the thermal conductivity (κ) of a *system* of carbyne chains to enable statistical averaging, subject to both variations in length and applied strain. Rather than equilibrium methods, the Müller-Plathe reverse perturbation method is used to obtain κ along the chain direction.

2. Methods

Herein we describe the computational methodology and underlying theory of the work, including the constructed molecular system, the basis for calculating thermal conductivity *via* reverse nonequilibrium molecular dynamics (RNEMD), and the atomistic modeling framework:

To enable a broader distribution of atomistic temperatures, enhanced stochastic sampling, and system averaging, we constructed a carbyne system consisting of *ten* independent carbyne chains, each chain containing 300 carbon atoms. The chains consist of alternate triple and single bonds, with initial equilibrium lengths of approximately 1.21 Å and 1.42 Å respectively, resulting in a total chain length on the order of 40 nm.

2.1. Thermal conductivity and reverse nonequilibrium molecular dynamics

Thermal conductivity is a property that measures the rate at which energy is transferred from two regions of a material that are held at different temperatures. For small temperature gradients, that is, in the realm of linear response theory, the thermal conductivity coefficient κ of a bulk material relates the heat flux vector J_0 to a spatial temperature gradient ∇T *via* Fourier's law:

$$\kappa = J_0 / \frac{dT}{dx} \quad (1a)$$

where $\nabla T = dT/dx$ in 1D. The Müller-Plathe reverse perturbation method, or Reverse Non-Equilibrium MD (RNEMD) was used to obtain κ along the chain direction, which is a simulation of experimental measurement. The Müller-Plathe method is a well-known approach to calculate thermal conductance due to its relative simple implementation [10]. The scheme offers several advantages such as compatibility with periodic boundary conditions, conservation of total energy and total linear momentum, and the sampling of a rapidly converging quantity (temperature gradient) rather than a slowly converging one (heat flux), as typically seen in equilibrium approaches, such as Green-Kubo methods [6]. In the Müller-Plathe approach, a constant-energy molecular dynamics simulation (a microcanonical or NVE ensemble) is performed and additional control is made through exchanging the momentum of one group of atoms (hot reservoir) to another (cold reservoir), depicted in Fig. 2. After achieving a steady state of the system, a temperature gradient (dT/dx) of the system can be computed and then the thermal conductance can be calculated by a simple rearrangement of Fourier's Law:

$$\kappa = \frac{Q}{2A} \left(\frac{1}{dT/dx} \right) \quad (1b)$$

where $J_0 = Q/2A$ is the known/applied heat flux, Q the heat flow rate (energy/time) and $2A$ the lateral area of the system (multiplied by two to account for the dissipation in two directions). Such an approach has been successfully implemented in carbon-dominated systems [11,12]. We note that here, the conductivity is highly dependent on the assumption of molecular cross-section

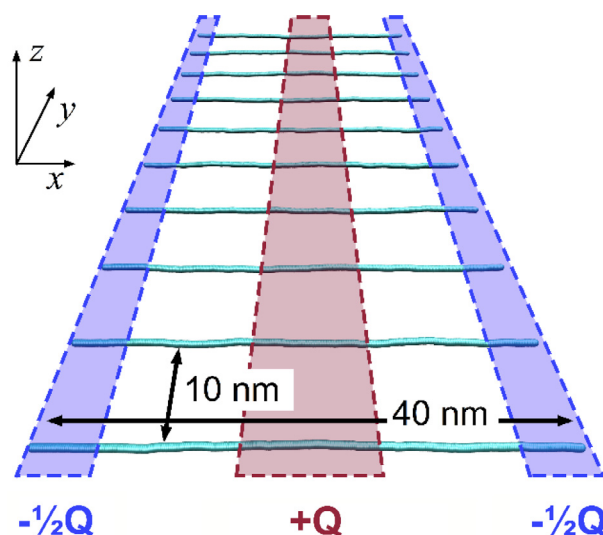


Fig. 2. Snapshot of full atomistic system after equilibration, prior to Müller-Plathe implementation. Ten independent carbyne chains approximate 40 nm in length. Middle section chosen as hot reservoir (+Q) and periodic ends chosen as cold reservoir (-Q total).

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