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ABSTRACT
Aiming to solve the heat dissipation problem of next generation energy-efficient nanoelectronics, we have explored the thermal transport behavior of monolayer silicon carbide nanoribbons (SiCNRs) using equilibrium molecular dynamics simulation based on Green-Kubo formalism. Our comprehensive analysis includes the calculation of thermal conductivity both for armchair and zigzag edged SiCNRs as a function of temperature, ribbon width, and length. At a temperature of 300 K, the thermal conductivity of 10 nm × 3 nm SiCNRs is found to be 23.92 ± 4.01 W/m K and 26.26 ± 4.18 W/m K for the armchair and zigzag direction, respectively. With the increase in temperature and length, a decreasing behavior of the thermal conductivity is observed for both directions of the SiCNRs, while the thermal conductivity increases with the increase in the ribbon width. Besides, to explain the size-dependent thermal transport phenomena, the acoustic phonon density of states is calculated using velocity autocorrelation of atoms. The variation of different low-frequency phonon modes validates the explored thermal conductivity at varying widths and lengths. These results would provide insight into and inspiration to design next-generation nanoelectronics with enhanced thermal efficiency using novel SiCNRs.

INTRODUCTION
In order to achieve superior device performance, the modern electronics industry is experiencing significant miniaturization of transistors which leads to high power densification. Nevertheless, this causes an enormous increase in heat current inside the device, which results in the decrease of device lifetime. Therefore, in order to sustain the optimal functioning temperature within the device, rapid and more efficient heat dissipation is becoming substantially critical in nanoelectronic packaging. In this respect, the analysis of novel nanostructured materials with extraordinary thermal properties is highly relevant. Of late, two-dimensional silicon carbides (2D-SiC) have attracted substantial attention due to their intriguing electronic, thermal, and mechanical properties. More recently, SiC nanoribbons (SiCNRs), one dimensional (1D) nanostrips of monolayer SiC, have gained great interest owing to their superior carrier doped spin adjusting, chemical decoration free half metallicity, nonmagnetic and ferromagnetic semiconducting property, high excitonic binding energy (~2.0 eV), and Bose–Einstein effect. Along with these exceptional properties, an intriguing thermal property is also anticipated from SiCNRs. However, although several studies have been carried out on the structural and electronic properties of SiCNRs, to the best of our knowledge, there has been no study on the thermal properties of SiCNRs. Earlier studies reported that the thermal conductivity of the 1D structures such as nanoribbons of graphene, stanene, h-BN, and
silicene shows a decreasing behavior with ribbon lengths and system temperatures. However, an increasing trend in thermal conductivity is noticed in these nanoribbons when the ribbon width is increased. The edges (armchair and zigzag) of the nanoribbons also demonstrate an intriguing effect on thermal conductivity. Furthermore, depending on the variation of the mass difference of the constituent’s atom and the phonon modes of nanoribbons, the thermal conductivity exhibits disparate behavior in different nanomaterial systems. A detailed understanding of the thermal properties of this prospective SiCNR is thus indispensable which confines the applicability of the ribbons in thermoelectric or heat management applications.

Hence, in this paper, we have characterized the thermal conductivity of SiCNRs using Green-Kubo (GK) formalism based equilibrium molecular dynamics (EMD) simulation. The classical Tersoff potential is employed to describe the atomicistic interaction of the SiCNR. The thermal conductivity of both armchair and zigzag configured SiCNRs is calculated at different temperatures ranging from 100 to 800 K. With a view of investigating the length dependence of thermal conductivity of SiCNRs, we varied the length from 10 to 25 nm with a constant width of 3 nm. In addition, the effect of the varying width on the thermal conductivity of the nanoribbon is also explored, taking a constant length of 10 nm, while the width was varied from 1 nm to 5 nm. A considerable effect is observed for the thermal conductivity of the SiCNRs upon variation of the ribbon length and width. Alongside rendering a deep intuition toward optimizing the thermal transport in the novel nanostructures, the modeling of the thermal property of SiCNRs accomplished in this article would inspire the effective design of this nanostructure-based thermo-electronic model.

**COMPUTATIONAL DETAILS**

In order to calculate the thermal conductivity of SiCNRs, we performed EMD simulations based on the GK method using the open-source large-scale atomic/molecular massively parallel simulator (LAMMPS). The EMD technique is considered more accurate for the calculation of thermal conductivity rather than its counterpart, i.e., nonequilibrium molecular dynamics (NEMD) simulation. In NEMD simulation, owing to the applied temperature gradient between the heat source and heat sink, a nonlinear effect is observed near the hot and cold regions, producing a strong scattering phenomenon. Hence, although EMD incurs more computational cost compared to NEMD and its simulation outputs are a bit susceptible to different factors, EMD is favorable for systems involving periodic boundary conditions. Furthermore, the EMD approach with the GK method removes the limitations of the size effect of NEMD and computes the thermal conductivity along all directions by using the total thermal conductivity tensor in conjunction with some additional constraints like the heat current auto-correlation function (HCACF). Considering these facts, we employed EMD simulation to model the thermal conductivity of SiCNRs. The HCACF of the statistical GK method is based on the linear response theorem wherein the thermal conductivity is calculated using the following equation:

\[
\kappa = \frac{1}{V R_T} \int_0^\infty \langle J_x(t) \cdot J_x(0) \rangle dt,
\]

where \(J_x\), \(V\), \(R_T\), and \(T\) represent the heat flux of the \(x\) component, the system volume [product of the sheet area and van der Waals thickness (3.5 Å)], the Boltzmann constant, and the system temperature, respectively. The ensemble average of the HCACF is presented by the \(\langle J_x(t) \cdot J_x(0) \rangle\) term, and \(r\) is the correlation period required for the reasonable decay of the HCACF.

For both armchair and zigzag edged SiCNRs, we considered a Si–C bond length of 0.179 nm in equilibrium. The armchair and zigzag edged SiCNRs are presented in Figs. 1(a) and 1(b), respectively. The Si–C bonding interactions are described using the classical Tersoff potential proposed by Tersoff. The conjugate gradient algorithm (CGA) was used to perform energy minimization of the system. By considering a time step of 0.5 fs, numerical integration (velocity-Verlet) is then applied on the system of atomic motion equations. The system was then thermalized from 100 K to 300 K using a Nose-Hoover thermostat for total time steps of \(3 \times 10^5\). At that time, to achieve thermal equilibrium, the Nose-Hoover thermostat was again used for \(3 \times 10^5\) time steps at 300 K. Later, we switched to NVE (constant volume, constant energy, and constant number of atoms) ensemble for \(2 \times 10^5\) time steps to conserve the total energy of the system. Finally, the thermal conductivity is calculated using the ensemble average of the HCACF. In this study, the heat-current information was noted for every five steps to attain the HCACFs by carrying out constant energy simulations. After that, the HCACF values were calculated by taking the average of the obtained ten HCACFs. Proper auto-correlation length is used to guarantee the sound decay of the normalized HCACF values. For different sizes of SiCNRs, different correlations are used for reasonable decay of the HCACF. At last, by fulfilling these conditions, thermal conductivity is calculated using Eq. (1).

In low dimensional materials, heat transportation is largely dependent on the phonon behaviors, including phonon-dispersion, phonon density of states (PDOS), phonon group velocities, etc. Therefore, understanding phonon properties is an important task to realize the reason of thermal transport variation under different conditions. Moreover, among optical and acoustic phonons, low frequency or acoustic phonon modes are responsible for thermal transport in nanoscale materials. Hence, in this work, to quantify the fact of thermal conductivity variation with SiCNR widths and lengths, we have calculated the acoustic phonon density of states.
(PDOS) of both armchair and zigzag SiCNRs. To perform this, the SiCNr is taken under equilibrium condition with NVT and NVE ensemble MD simulation. Finally, the acoustic PDOS is calculated using the Fourier transform of the velocity auto-correlation function of atoms. The phonon density of states is calculated with the velocity auto-correlation function as

\[ F(\omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dt e^{i\omega t} \frac{\langle v(0) \cdot v(t) \rangle}{\langle v(0) \cdot v(0) \rangle} \]  

(2)

where, \( F(\omega) \) denotes the phonon spectrum, \( \omega \) is the vibrational wave number, \( v(t) \) and \( v(0) \) represent the velocity of the particle at time \( t \) and time 0, respectively, and the brackets denote averages over atoms and time origins.

RESULTS AND DISCUSSION

To investigate the temperature dependence on the thermal conductivity of SiCNRs, we varied the temperature from 100 K to 800 K, while the dimension of the SiCNr was taken as 10 nm \( \times \) 3 nm (length \( \times \) width). At room temperature (300 K), the calculated thermal conductivity of the armchair edge SiCNr is found to be 23.92 ± 4.01 W/m K, whereas it is 26.26 ± 4.18 W/m K for the zigzag edge SiCNr. Recently, Islam et al.\(^6\) reported a room temperature thermal conductivity of \( \sim 313 \) W/m K for a monolayer SiC sheet using NEMD simulation where they considered infinite length 2D-SiC with a sheet thickness of 3.50 Å. In contrast to the single layered SiCNr, as one of the dimensions (width) is reduced, a far less thermal conductivity is anticipated in the nanoribbons.\(^7\)

The lowering of the thermal conductivity value with nanostructuring thus conforms well to our obtained results. Quite the reverse, Guo et al.\(^8\) obtained a thermal conductivity of \( \sim 16.76 \) W/m K for monolayer SiC using the Boltzmann transport equation which is even less than the thermal conductivity of SiCNRs obtained in the present study. The thickness they considered (18 Å) was much higher compared to that considered in the present study and by Islam et al.,\(^9\) which might be the possible reason for such variation. Moreover, our estimated thermal conductivities of SiCNRs for both directions are pretty higher than the thermal conductivity of the nanomaterials like GaN (14.9 W/m K),\(^8\) ZnO (4.5 W/m K),\(^8\) stanene (11.6 W/m K),\(^9\) and stanene nanoribbon (\( \sim 0.95 \) W/m k for the zigzag edge and \( \sim 0.9 \) W/m k for the armchair edge),\(^8\) whereas the values are comparable to a silicene nanosheet (\( \sim 20 \) W/m K).\(^10\)

On the other hand, the obtained thermal conductivity values in this work are considerably lower than the thermal conductivity of the graphene nanoribbon (3207 W/m K),\(^11\) boron-nitride nanoribbon (649 W/m K),\(^12\) monolayer AlN (\( \sim 264.1 \) W/m K),\(^13\) monolayer MoS\(_2\) (\( \sim 34.5 \) W/m K).\(^12\) The difference in the thermal conductivity of SiCNRs with respect to the aforementioned nanomaterials can be attributed to the variations in atomic masses, phonon group velocities, Debye temperatures, and phonon scattering rates. Specifically, in binary systems, the estimated value of thermal conductivity largely depends on the mass ratio of the constituent’s atoms.\(^14\) A lower value of thermal conductivity might arise from the fact of significant phonon band gaps between acoustic and optic phonons and the different nature of the intrinsic scattering processes in large mass ratio compounds compared to those with small mass ratios.\(^14\)

Consequently, in the SiC system, significant phonon band gaps are reported between the acoustic and optic phonons,\(^15\) which cause a lower value of thermal conductivity compared to the single atom system.\(^15\) In addition, owing to the strong polarization effect and strong phonon scattering effect, a lower phonon group velocity might be present, which further generates a lower Debye temperature responsible for the lower value of thermal conductivity of SiCNRs.

Moreover, for monolayer SiC, the contribution of high-frequency optical mode phonons in heat transport is almost negligible up to room temperature. Among the acoustic phonon branches, the flexural acoustic (FA) mode contribution also tends to become smaller when the temperature is increased from room temperature to a higher temperature. Hence, due to the reduced contribution of FA mode phonons as well as the negligible effect of high-frequency optical mode phonons, the SiCNr shows a significantly lower value of thermal conductivity compared to graphene nanoribbon (GNR), h-BNNR, monolayer AlN, and MoS\(_2\).

Figure 2 represents the thermal conductivity of SiCNRs as a function of temperature for armchair and zigzag directions. As the figure depicts, the thermal conductivity of SiCNr decreases with the increase in temperature, while the decreasing rates are slightly different for the two directions. Nanomaterials like stanene nanoribbons,\(^9\) silicene,\(^11\) germanene,\(^12\) GNR,\(^9\) and h-BNNR\(^11\) also exhibit a similar decreasing trend of thermal conductivity with respect to temperature. Moreover, above room temperature, the thermal conductivity deviates from the normal 1/T law and shows an anomalous decreasing behavior for both armchair and zigzag SiCNRs. The drooping behavior of thermal conductivity may occur due to the enlargement of nonlinear thermal resistivity created by phonon-phonon interactions over the boundary scattering.

**FIG. 2** Temperature dependent thermal conductivity of SiCNRs with a width of 3 nm and a length of 10 nm; inset shows the comparison of the decaying trend of HCACFs between the armchair and zigzag SiCNRs at 300 K.
mechanism at an elevated temperature. In addition, the anomalous thermal conductivity reduction trend in this SiCNR may also occur due to the mass variation induced phonon band gaps and the different nature of the intrinsic scattering processes for heat-carrying acoustic phonons. Calculated maximum and minimum thermal conductivity for armchair SiCNR is $26.23 \pm 5.84$ W/m K and $12.36 \pm 5.86$ W/m K at temperatures 100 K and 800 K, respectively, while along the zigzag direction, the thermal conductivity of SiCNRs is calculated to be $30.75 \pm 3.27$ W/m K and $13.94 \pm 3.48$ W/m K at temperatures 100 K and 800 K, respectively. Thus, the thermal conductivity of zigzag directed SiCNRs is a little higher than the thermal conductivity of armchair SiCNRs. A similar trend is also observed in the thermal transport analysis of GNRs, carbon nanotubes, stanene nanotubes, stanene nanoribbons, and h-BNNRs. Nonetheless, at high temperature (~800 K), the thermal conductivity values for the zigzag and armchair direction of the SiCNR were very close to each other. This phenomenon is due to relatively greater phonon group velocities of the armchair directed SiCNR compared to the zigzag direction at high temperature. Total energies at different temperatures are shown in Fig. 3 with the aim to validate the simulations performed in this study at different temperatures and also to confirm the stability of the SiCNR. As the figure reflects, the energy fluctuations were insignificant; thus the firmness of the SiCNR configuration is confirmed.

In order to explain the influence of increasing temperature on the thermal conductivity of both armchair and zigzag SiCNRs, a reasonable decay of the HCACF necessary for the calculation of the thermal conductivity using GK formalism is presented in Fig. 4. The decreasing behavior of the thermal conductivity of SiCNRs with an increase of temperature is noticed in the decaying rates of HCACFs. With increasing temperature, the phonon-phonon scattering, specifically, the Umklapp limited phonon scattering, also increases owing to the amassed number of acoustic phonons. Accordingly, when the temperature is increased to a higher value, the HCACF profile declines to zero in a very short time. As a result, the thermal conductivity of SiCNRs follows a decreasing trend with the increase in temperature. The comparison of the decaying trend of HCACFs between the armchair and zigzag SiCNRs at 300 K is shown in the inset of Fig. 2 which again confirms the higher value of thermal conductivity of zigzag SiCNRs compared to armchair SiCNRs for a certain temperature.

The change in the thermal conductivity of SiCNRs upon the variation of ribbon width for both of the armchair and zigzag configurations is shown in Fig. 5 where the ribbon width is varied from 1 nm to 5 nm with a constant length of 10 nm. For the armchair directed SiCNR, the obtained thermal conductivity values are $13.89 \pm 1.80$ W/m K and $29.68 \pm 1.88$ W/m K for 1 nm and 5 nm ribbon widths. Figure 4 shows the envelopes of normalized HCACFs for (a) armchair and (b) zigzag SiCNRs at different temperatures. The ribbon width and length are considered to be 3 nm and 10 nm, respectively.
width, respectively. In contrast, the computed thermal conductivity values are 19.65 $\pm$ 2.91 W/m K for 1 nm width and 33.04 $\pm$ 2.78 W/m K for 5 nm ribbon width for the zigzag configuration. As Fig. 5 reflects, the thermal conductivity increases monotonically with the increase in ribbon width. In addition, zigzag configured SiCNRs exhibit a higher value of thermal conductivity compared to an armchair configuration with the increase in ribbon width. Akin to SiCNRs, the increasing behavior of thermal conductivity with increasing width in both directions is also reported for nanostructures like GNRs\textsuperscript{23} and h-BNNRs.\textsuperscript{52} Two mechanisms, the boundary scattering or edge localized phonon scattering and the Umklapp limited phonon scattering, are considered as the principal reasons for this type of thermal transport behavior with respect to width.\textsuperscript{20–22} Each of these mechanisms separately tends to reduce the thermal conductivity of SiCNRs. Nevertheless, with the increase in ribbon width, these two mechanisms behave opposite to each other, i.e., the boundary scattering effect declines but at the same time the Umklapp limited phonon scattering increases owing to an increased number of phonons. Therefore, due to the smaller ribbon width initially considered, edge localized phonon scattering primarily governs the thermal conductivity of SiCNRs. However, with an increased ribbon width, the edge localized phonon scattering effect is suppressed compared to the Umklapp limited phonon scattering, causing improved thermal conductivity\textsuperscript{23,54} with ribbon width. When the ribbon width is further increased to a greater value, more numbers of phonons are available for strengthening the Umklapp limited phonon scattering effect. Accordingly, the proportion of the increase in thermal conductivity is rapid initially and diminishes gradually when the ribbon width increases to a larger extent. This behavior is in close agreement with the formerly reported studies on thermal transportation of different nanoribbons.\textsuperscript{23,55–57}

To ensure good convergence of the GK formalism based thermal conductivity calculation of SiCNRs, a reasonable decay for the HCACF for both the armchair and zigzag direction was maintained in our study [Figs. 6(a) and 6(b)]. Moreover, this HCACF calculation for varying ribbon width can be an indicator to explain the width dependent thermal conductivity of SiCNRs. As depicted in Figs. 6(a) and 6(b), the decay rate of the envelopes of normalized HCACFs is higher at 1 nm width and lower at 5 nm width for both SiCNR structures. The acoustic PDOS of SiCNRs for a varying width having a constant length of 10 nm is also presented in Figs. 7(a) and 7(b) for both armchair and zigzag configuration, respectively, to shed more light on the width dependent thermal conductivity of SiCNRs. As the figures suggest, the magnitude of the dominant peaks for 5 nm width is higher than that for 1 nm width. This can be attributed to the increased availability of low-frequency acoustic phonons with increasing ribbon width, causing more phonons to get active for thermal transport. Owing to the higher phonon group velocities of low-frequency phonons as well as their lower scattering rate, this type of augmented peaks is observed in the acoustic PDOS curves. Hence, the thermal conductivity of SiCNRs increases sharply with the increase in ribbon width. In addition, the acoustic PDOS of SiC is limited to the 20 THz frequency region of the phonon spectrum, whereas the range of acoustic PDOS of GNR and h-BNNR is 50–60 THz.\textsuperscript{21,23,24,58,59} This variation in the acoustic range of the phonon spectrum of SiCNRs with respect to GNR and h-BNNR further signifies the lower thermal conductivity of SiCNRs with respect to GNR and h-BNNRs and indicates the reliability of our simulation.
Figure 8 represents the thermal conductivity of SiCNRs as a function of length. For both armchair and zigzag configurations, the length is varied from 10 nm to 25 nm with a fixed width of 3 nm. For a length of 10 nm, the thermal conductivity of armchair and zigzag SiCNRs is found to be $23.92 \pm 4.01 \text{ W/m K}$ and $26.26 \pm 4.18 \text{ W/m K}$, respectively. However, the value decreased to $16.54 \pm 5.64 \text{ W/m K}$ and $18.85 \pm 4.88 \text{ W/m K}$ for 25 nm length. Therefore, with increasing length, the thermal conductivity of SiCNRs decreases in a monotonic way for both armchair and zigzag directions, and the zigzag directed SiCNR is less affected than the armchair direction for all considered lengths. Besides, thermal conductivity results for a varying length follow a similar trend to the study of GNRs by Mahdizadeh et al., graphene, silicon and silicene by Wang et al., and h-BN by Noshin et al. The decaying behavior of thermal conductivity of SiCNRs with respect to length can be explained using the HCACF profiles for the two directions, as shown in Figs. 9(a) and 9(b). With the increase in ribbon length, increased edge localized phonon scattering is observed which results in a faster decay of the HCACF profile. A recent study on GNR, h-BNNR, silicene, and graphene supports this nature of the HCACF profile with increasing ribbon length.

The convergence nature of the computed HCACF based length dependence thermal conductivity of SiCNRs can be explained with...
the help of phonon mode contributions.\textsuperscript{14,60,61} According to Guo et al., among the three acoustic phonon modes up to room temperature, the contribution from the ZA modes is maximum, and a quadratic dispersion behavior is observed in the phonon dispersion curve. Furthermore, near the $\Gamma$ point, the group velocity of the ZA mode phonon tends to be zero. Consequently, low-frequency ZA phonon modes cause the scattering of other acoustic heat carriers and thereby results in lowering and converging of the thermal conductivity of the SiCNRs. Donadio et al.\textsuperscript{11} also reported a similar effect of the flexural phonon modes in the convergence of length-dependent thermal conductivity of carbon nanotubes (CNTs). This low-frequency FA mode phonon mainly acts as a scattering element of the heat carriers\textsuperscript{7} and is responsible for the convergence of thermal conductivity of CNTs with varying lengths.

To elucidate the length dependence of the thermal conductivity of SiCNRs, acoustic PDOS of the armchair and zigzag SiCNRs for varying lengths with a fixed width of 3 nm is shown in Figs. 10(a) and 10(b), respectively. As the figures suggest, with the increase in ribbon length, the peaks of the phonon at the higher energy regions do not increase sharply but rather show a suppressing tendency with increasing length. This fact can be described easily using edge localized phonon scattering. Phonon population increases with the increase in ribbon length. However, as the width is fixed, edge localized phonon scattering increases in the whole length of the ribbon. Besides, due to the increased phonon population with increasing length, an enormous Umklapp limited phonon scattering also occur. These two scatterings cause a negative effect on the heat transport of SiCNRs, i.e., a reduction in thermal conductivity with increasing ribbon length and generate suppressing type acoustic peaks. Furthermore, according to Guo et al.,\textsuperscript{7} as FA mode phonons control the heat transport up to 300 K and show quadratic dispersion behavior near the $\Gamma$ point, the low energy region peaks prominently. Nonetheless, as it also acts as scattering elements, it helps lessen the thermal conductivity with increase in ribbon length.

\section*{CONCLUSION}

In conclusion, the thermal conductivity of both armchair and zigzag SiCNRs are studied using EMD simulation. The impacts of temperature, width, and length variation on thermal conductivity are explored. Extraordinary thermal properties are found from these investigations. The thermal conductivity shows a decreasing behavior with temperature and length. However, an increasing nature is observed when the ribbon width is increased. To elucidate the reason for the variation of thermal conductivity at a different temperature, ribbon length, and ribbon width, we have calculated acoustic PDOS, HCACF, and total energies of the system. The variation in acoustic PDOS and HCACF shows intriguing results with a variation in the structure. Moreover, the convergence and negative value of the total energy of a particular structure further confirms the stability and validity of our simulation results. These findings will be beneficial in designing SiCN based nanoelectronic devices with superior thermal performances.

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