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Carbon-nitride 2D nanostructures: Thermal conductivity and interfacial thermal conductance with the silica substrate

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Abstract

The rate of heat dissipation from a 2D nanostructure strongly depends on the interfacial thermal conductance with its substrate. In this paper, the interfacial thermal conductance of carbon-nitride 2D nanostructures (C_3N , C_2N , C_3N_4 's) with silica substrates was investigated using transient molecular dynamics simulations. It was found that a 2D nanostructure with higher thermal conductivity, has a lower value of interfacial thermal conductance with the silica substrate. The thermal conductivity of suspended carbon-nitride 2D nanostructures was also calculated using Green-Kubo formalism and compared with that of graphene as a reference structure. It was found that the thermal conductivities of C_3N , C_2N , C_3N_4 (s-triazine) and C_3N_4 (tri-triazine) are respectively 62%, 4%, 4% and 2% that of graphene; while their interfacial thermal conductances with silica are 171%, 113%, 188% and 212% that of graphene. This different behaviors of the thermal conductivity and the interfacial thermal conductance with the substrate can be important in the thermal management of carbon-nitride 2D nanostructures in nanoelectronics.

1. Introduction

Carbon-nitride 2D nanostructures have non-zero electronic energy band-gap (~ 2 eV) in contrast to mono-elemental 2D structures such as graphene, silicene, germanen, and stanine [1]. This brilliant property of carbon-nitride 2D nanostructures makes them excellent

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candidates for future applications in electronic devices such as transistors or optic diodes [2,3]. Therefore, several studies have been recently targeting thermophysical properties of carbon-nitride 2D nanostructures. By performing first-principle calculations, structural, phononic, thermal and mechanical properties of nitrogenated holey graphene (C_2N) as one of the essential carbon-nitride 2D nanostructures have been reported [4,5]. Besides, by performing first-principle calculations, nonequilibrium molecular dynamics and equilibrium molecular dynamics simulations, the thermal conductivity of C_2N has been calculated and a dramatically lower value than the one of graphene was obtained [4,6,7]. Nonequilibrium Green's function shows a more efficient thermoelectric behavior of C_2N compared to the one of graphene [8]. Another carbon-nitride 2D nanostructure C_3N with a structure similar to regularly nitrogen-doped graphene also indicates high mechanical strength and phononic thermal conductivity [9–13]. Other carbon-nitride 2D nanostructures named as C_3N_4 recently synthesized in the two forms of s-triazine-based and tri-triazine-based show low thermal conductivity but high mechanical strength property [1,14,15].

Although the properties of carbon-nitride 2D nanostructures make them appropriate in electronic applications, they should be in contact with a substrate such as SiO_2 in electronic devices. In those latter, generated heat leads to the temperature rise and consequently decrease life time and effectiveness of electronic devices. The rate of heat dissipation strongly depends on the interfacial thermal conductance between a 2D nanostructure and its substrate. Thus, heat transfer analysis between these two bodies is crucial in their optimal thermal design. Although several studies on the calculation of interfacial thermal conductance between silica or silicon substrate and 2D nanostructures such as graphene, silicene, phosphorene and MoS_2 have been published, the interfacial thermal conductance between carbon-nitride 2D nanostructures and SiO_2 has not yet been reported [16–19].

In this study, we first calculate the thermal conductivities of four carbon-nitride 2D nanostructures as C_3N , C_2N , C_3N_4 (s-triazine) and C_3N_4 (tri-triazine) by performing equilibrium molecular dynamics simulations. By using the same potential functions and MD method, the thermal conductivity of those structures can be accurately compared in contrast to previous studies. Then by simulating carbon-nitride 2D nanostructures deposited on a silica substrate, we report the interfacial thermal conductance using a transient molecular dynamics method inspired from the experimental pump-probe technique. Finally, the dependency of the thermal conductivity and the interfacial thermal conductance to the substrate temperature will be examined.

2. Molecular dynamics simulation model

The atomistic geometries of studied carbon-nitride 2D nanostructures are shown in Figure 1. The simulated structures are squares 30nm in edge with periodic boundary conditions in the two planar directions. This size is enough to ensure that MD results are not sensitive to the chosen dimensions. Tersoff potential function is used to describe carbon (C) and nitrogen (N) interactions in 2D nanostructures and also between silicon (Si) and oxygen (O) in the silica substrate [20,21]. The former potential was widely used to study the thermal transport in nitrogen-doped graphene[22–25]. For Van der Waals interactions between 2D nanostructures and substrate, Lennard-Jones potential function is employed with coefficients presented in Table 1. The coefficients are extracted from the UFF table [26]. The time-step for running the simulations for graphene, C_3N and C_2N nanostructures was set to 1fs; while for C_3N_4 nanostructures it was set to be 0.1 fs to stabilize the system. LAMMPS package was employed to perform all the simulations.

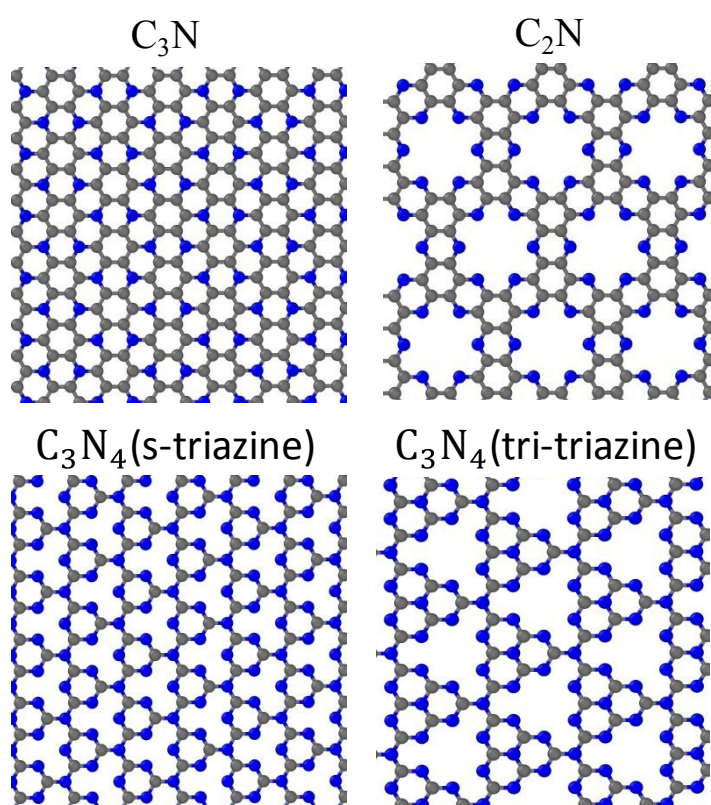


Figure 1: Atomistic configuration of carbon-nitride 2D nanostructures. Gray and blue atoms are carbon and nitrogen, respectively.

Table 1. Lennard-Jones potential coefficients for van der Waals interactions [26].

	ε (meV)	σ (Å)
C-Si	8.91	3.33
N-Si	7.16	3.53
C-O	3.44	3.00
N-O	2.76	3.19

3. Results and Discussion

3.1 Thermal conductivity

The thermal conductivity was calculated from the Green-Kubo relation as follows:

$$\kappa = \frac{1}{k_B T^2} \int_0^\infty \langle q_x(t) q_x(0) \rangle dt \quad (1)$$

where k_B is the Boltzmann constant, T is the equilibrium temperature and q_x refers to the instantaneous heat flux in the system. Figure 2 reports the thermal conductivity of carbon-nitride 2D nanostructures by replacing the upper integration bound by a variable time limit in equation 1. For comparison, results were normalized by the thermal conductivity of graphene ($\kappa_{Gr} = 847.7$ W/mK) at $T=300$ K. This value is in agreement with the EMD result reported by Pereira and Donadio [27]. The thermal conductivities of carbon-nitride 2D nanostructures display considerable differences between each other, so that the thermal conductivities of C_3N , C_2N , C_3N_4 (s-triazine) and C_3N_4 (tri-triazine) structures are respectively 62%, 4.4%, 4.1% and 2.2% that of graphene. Those discrepancies might be due to the differences in lattice structures with graphene [28]. This might explain why C_3N has the largest thermal conductivity which has a honeycomb lattice structure similar to graphene.

In order to better understand the differences in the thermal conductivities, the phonon density of states [29,30] was reported in figure 3. The phonon spectra of the graphene and C_3N structure are similar except that the maximal phonon frequency is lower in C_3N . However, the phonon spectrum of C_2N and C_3N_4 structures differ from the ones of graphene and C_3N which reveals phonon softening and justifies the lower conductivities of C_2N and C_3N_4 structures compared

to those of graphene and C_3N . Moreover, C_2N and C_3N_4 have less atoms per unit surface and therefore a smaller density of states and a smaller thermal conductivity. View Article Online
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In order to probe the dependency of the thermal conductivity of carbon-nitride 2D nanostructures to temperature variations, the thermal conductivity was calculated in the temperature range of 200-700 K as shown in figure 4. The results were normalized to the thermal conductivity of graphene at $T=200$ K. The thermal conductivity of all structures decreases when the temperature increases, which is due to the rise of the phonon-phonon scattering rate [31]. The largest reduction (77%) occurs for the thermal conductivity of graphene, and the smallest one (63%) corresponds to C_3N and C_3N_4 (s-triazine). However, the rate of thermal conductivity decrease as a function of temperature is almost the same for all structures.

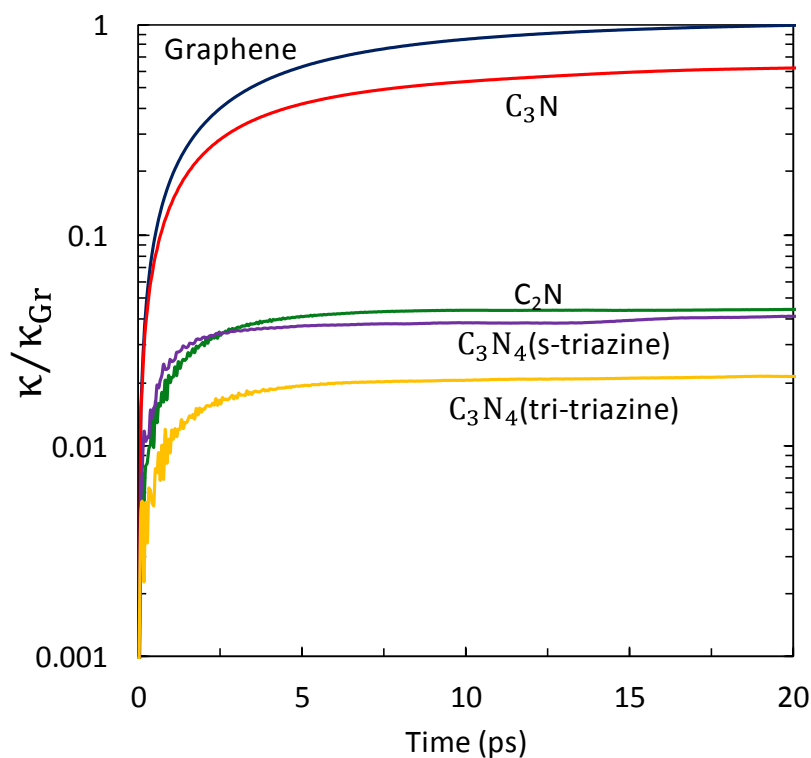


Figure 2: Time accumulated thermal conductivity of carbon-nitride 2D nanostructures computed with equation (1) and normalized by the thermal conductivity of graphene.

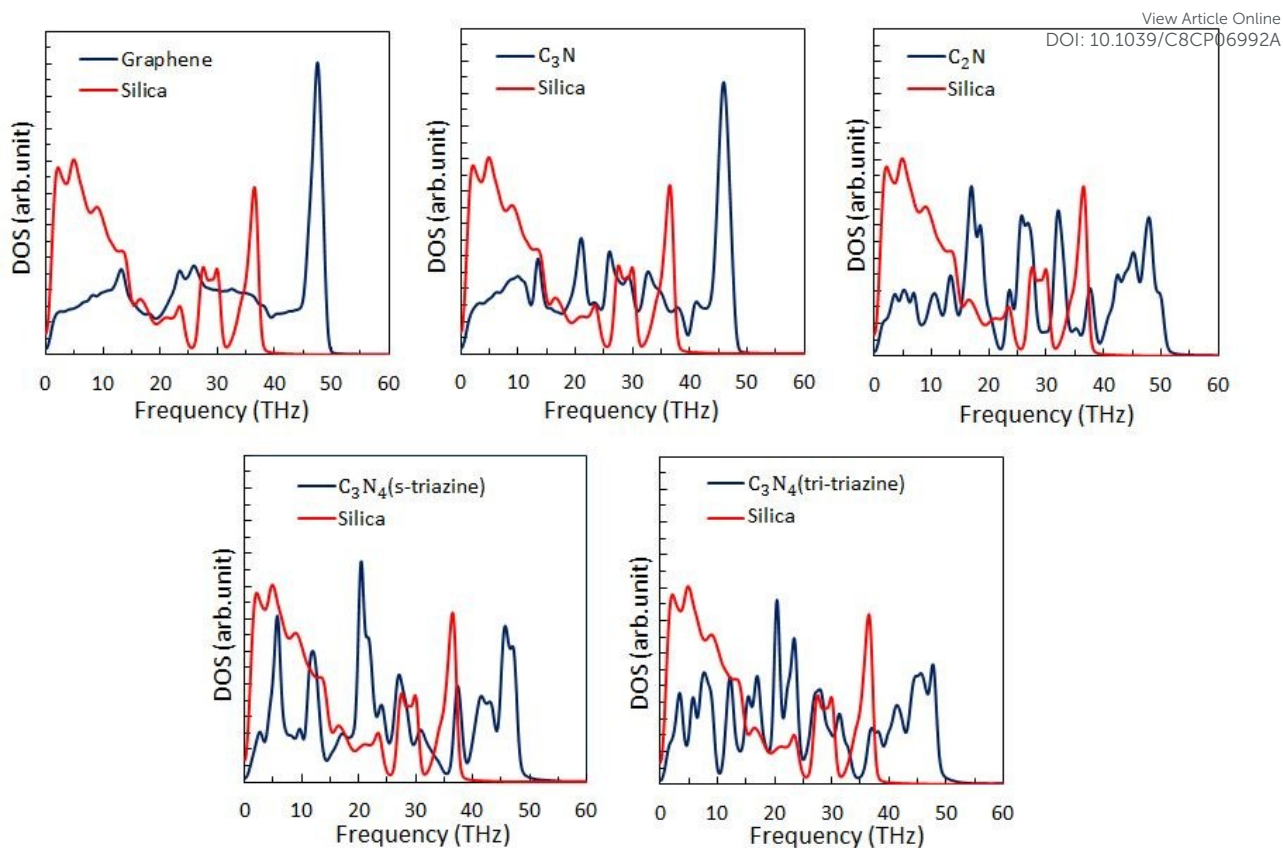


Figure 3: Phonon densities of states of carbon-nitride 2D nanostructures and of the silica substrate.

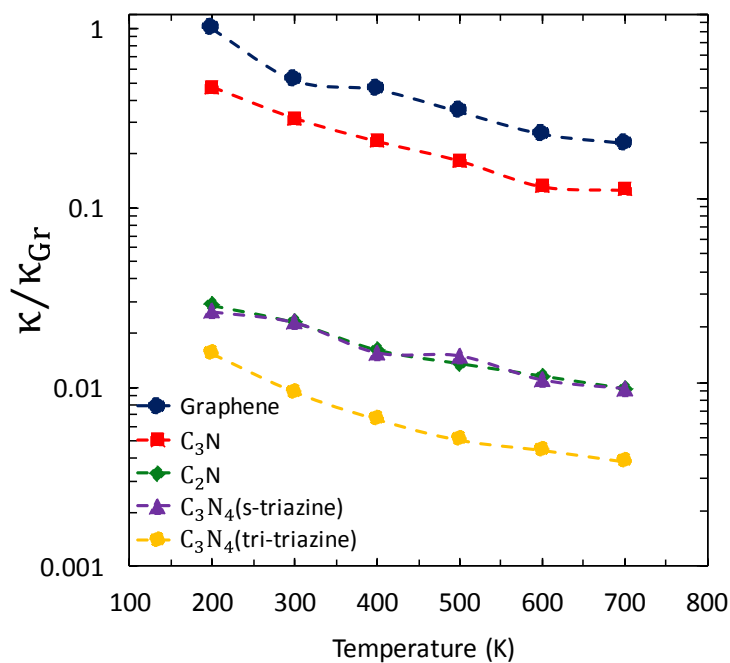


Figure 4: Thermal conductivity of carbon-nitride 2D nanostructures with respect to temperature normalized by the thermal conductivity of graphene at $T=200\text{K}$.

3.2 Interfacial thermal conductance

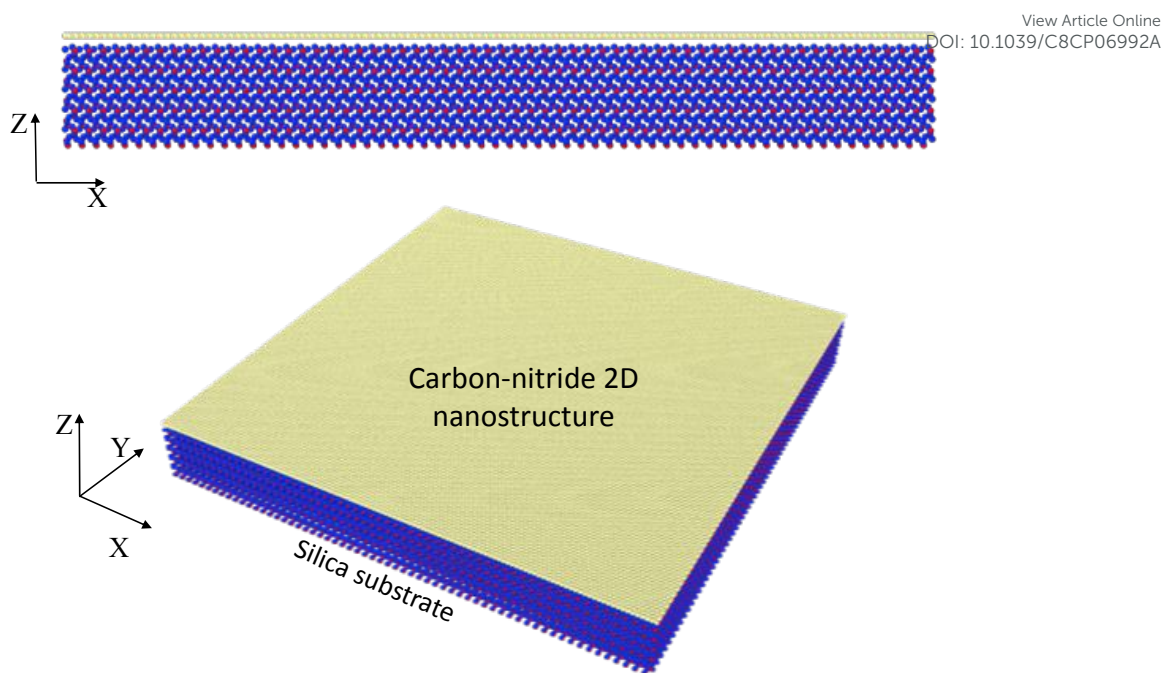
Figure 5 shows the atomistic simulation of a carbon-nitride 2D nanostructure deposited on a substrate. There are a lot of MD techniques to compute the interfacial thermal conductance [32–36]. In this work, a transient technique inspired by an experimental method was performed. To this aim, the initial temperature of the carbon-nitride 2D nanostructure was set to 500K, while the temperature of the substrate was maintained at 300K using N ose-Hoover thermostats. Then by switching off the thermostats, the temperature changes of both materials and the total energy reduction of the 2D nanostructure were recorded as reported for C₂N in figure 6a. The energy balance equation for the carbon-nitride 2D nanostructure can be considered as follows:

$$\frac{\partial E_t}{\partial t} = -GA(T_{CN} - T_{Si}) \quad (2)$$

where E_t is the total energy of the 2D system and T_{CN} is its temperature. T_{Si} refers to the temperature of the silica substrate with thickness of 0.5nm which is equal to the cut-off distance of carbon and oxygen atomic interaction subtracted by the gap distance between carbon-nitride structure and the silica substrate. G is the interfacial thermal conductance and A refers to the surface area of the interface. By integrating equation 2 with respect to time, G was fitted to the molecular dynamics results. Figure 6b shows the variation of the total energy of C₂N with respect to the integral of the MD computed temperature difference between C₂N and the silica substrate. It can be seen that the slope of the curve is almost constant in the considerable portion of the curve, which supports the assumption of constant interfacial thermal conductance during the thermal relaxation.

Results of the interfacial thermal conductance for different carbon-nitride 2D nanostructures and graphene are shown in figure 7. The changes in the interfacial thermal conductance value for different structures contrast with the ones of the thermal conductivities. The higher the thermal conductivity of a structure, the smaller its interfacial thermal conductivity.

In order to better understand the differences in the interfacial thermal conductances, the phonon density of states of carbon-nitride 2D nanostructures and silica substrate are represented in figure 3. The densities of states of graphene and silica are in good agreement with those of previous studies [37]. The dissimilarity between graphene and C₃N with their silica substrates are significantly more marked than the one of other carbon-nitride 2D nanostructures and their silica substrates. Expectedly, a larger difference between phonon spectra leads to a lower phonon coupling between two structures and consequently, a lower interfacial thermal conductance.



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Figure 5: Atomistic configurations (top and perspective views) of a carbon-nitride 2D nanostructure deposited on a silica substrate.

In order to determine the dependence of the interfacial thermal conductance between carbon-nitride 2D nanostructures and a silica substrate to the temperature variations of the substrate, the interfacial thermal conductance was calculated in the temperature range of 200-700 K as shown in figure 8. The interfacial thermal conductance of all structures increases when the temperature increases due to the enhancement of anharmonic phonon coupling of the two systems[37,38]. The largest enhancement (111% and 100%) corresponds to the interfacial thermal conductance of graphene and C_3N , and the smallest one (76 %) is computed in C_2N structure. However, all the interfacial thermal conductance variations with respect to temperature are in the same range.

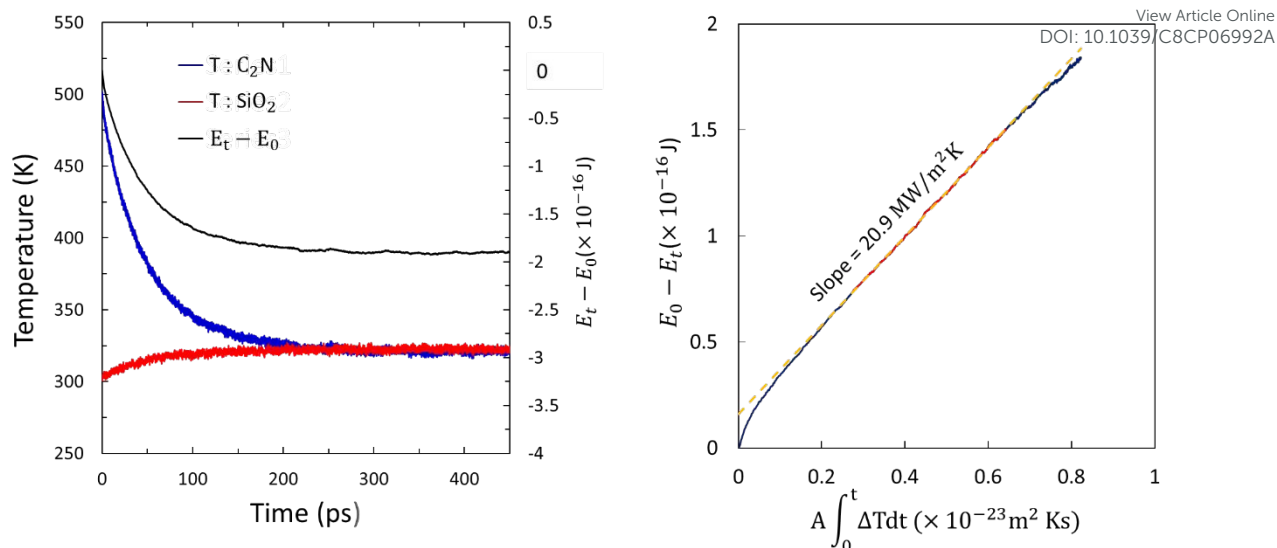


Figure 6: (a) Time evolutions of C_2N total energy as well as of C_2N and silica substrate temperatures during thermal relaxation. (b) Variation of the total energy of C_2N with respect to the integral of the temperature difference between C_2N and silica substrate. The slope of the latter curve directly yields the interfacial thermal conductance as deduced from equation 1.

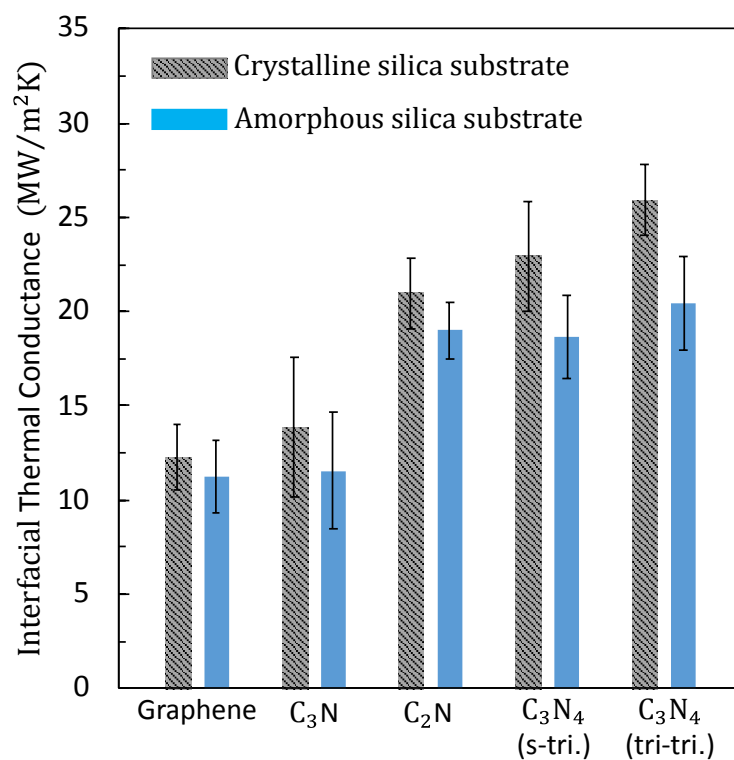


Figure 7: Interfacial thermal conductance between carbon-nitride 2D nanostructures and the silica substrate with crystalline and amorphous forms

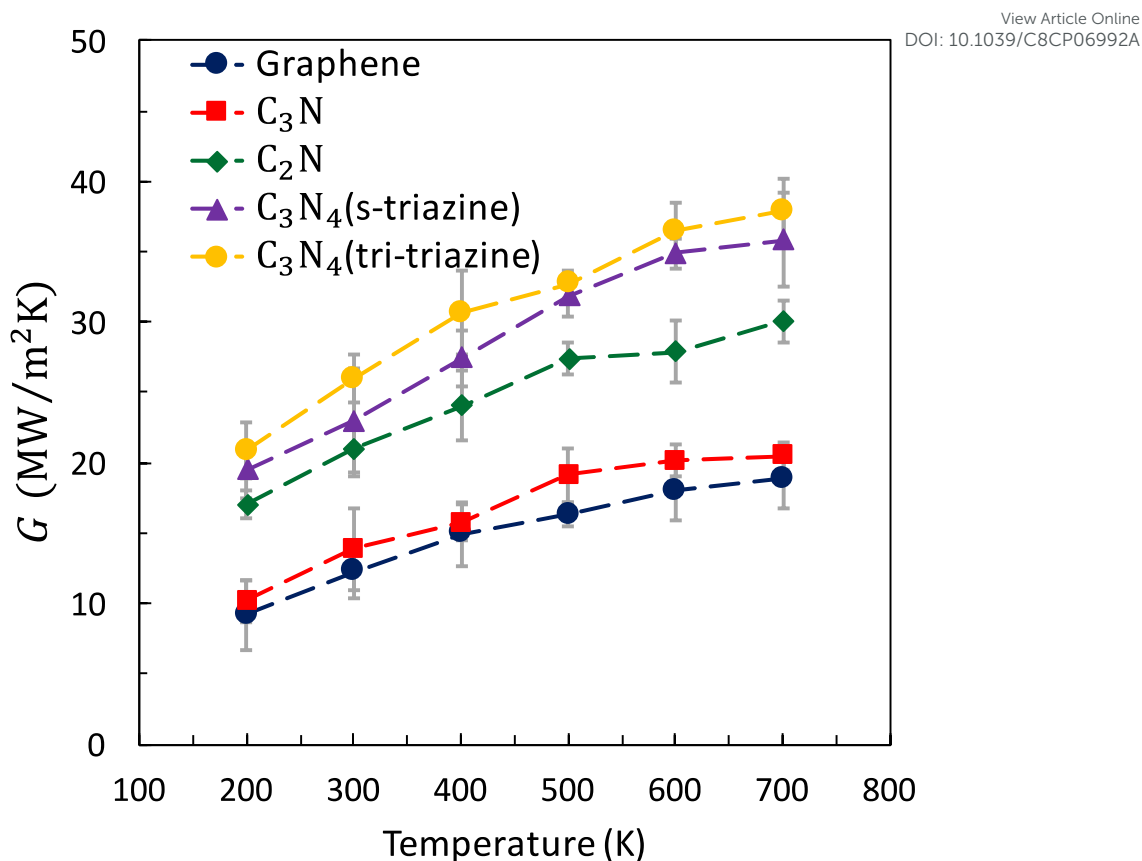


Figure 8: Interfacial thermal conductance of carbon-nitride 2D nanostructures with respect to the substrate initial temperature.

4. Summary

In this study, the thermal conductivities of carbon-nitride 2D nanostructures and their interfacial thermal conductance with the silica substrate were calculated with molecular dynamic simulation. The results showed that the thermal conductivities of these nanostructures are significantly different, so that the thermal conductivity of the structures C₃N, C₂N, C₃N₄ (s-triazine) and C₃N₄ (tri-triazine) is equal to 62%, 4.4%, 4.1% and 2.2% that of graphene at T=300K, respectively. Therefore, it can be concluded that the presence of holes in C₂N, C₃N₄ (s-triazine) and C₃N₄ (tri-triazine) structures has led to a sharp decrease in their thermal conductivities. Interestingly, the behavior of the interfacial thermal conductance of these structures with the silica substrate is contrasting the one of their thermal conductivities in the suspended films. The structure with higher thermal conductivity has lower interfacial thermal conductance with the silica substrate. Also, the sensitivity of the thermal conductivity and of the interfacial thermal conductance to the temperature was investigated. It was shown that their sensitivity is lower than that of graphene. The proposed understanding of the thermal

behaviour of carbon nitride 2D nanostructures is promoting this material for the thermal management of micro/nano opto/electronic devices.

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