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# Interfacial thermal conductance in graphene/black phosphorus heterogeneous structures



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Yang Chen<sup>a</sup>, Yingyan Zhang<sup>c</sup>, Kun Cai<sup>a</sup>, Jinwu Jiang<sup>d</sup>, Jin-Cheng Zheng<sup>e</sup>, Junhua Zhao<sup>b,\*</sup>, Ning Wei<sup>a,\*\*</sup>

<sup>a</sup> College of Water Resources and Architectural Engineering, Northwest A&F University, 712100 Yangling, China

<sup>b</sup> Jiangsu Key Laboratory of Advanced Food Manufacturing Equipment and Technology, Jiangnan University, 214122 Wuxi, China

<sup>c</sup> School of Computing, Engineering and Mathematics, Western Sydney University, Penrith, NSW 2751, Australia

<sup>d</sup> Shanghai Institute of Applied Mathematics and Mechanics, Shanghai University, Shanghai, China

<sup>e</sup> Department of Physics, Xiamen University, 361005 Xiamen, China

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#### ABSTRACT

Graphene, as a passivation layer, can be used to protect the black phosphorus (BP) from the chemical reaction with surrounding oxygen and water. However, BP and graphene heterostructures have low efficiency of heat dissipation due to its intrinsic high thermal resistance at the interfaces. The accumulated energy from Joule heat has to be removed efficiently to avoid the malfunction of the devices. Therefore, it is of significance to investigate the interfacial thermal dissipation properties and manipulate the properties by interfacial engineering on demand. In this work, the interfacial thermal conductance between few-layer BP and graphene is studied extensively using molecular dynamics simulations. Two important parameters,  $P_{cr}$ , the critical heat power density of maintaining thermal stability, and  $P_{max}$ , the maximum heat power density with which the system can be loaded, are identified. Our results show that interfacial thermal conductance can be effectively tuned in a wide range by external strains and interfacial defects. The compressive strain can enhance the interfacial thermal conductance by one order of magnitude, while interface defects give a two-fold increase. These findings could provide guidelines in heat dissipation and interfacial engineering for thermal conductance manipulation of BP-graphene heat of the stratemation of the devices.

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#### 1. Introduction

Black phosphorous (BP) has stimulated tremendous research interest recently due to its outstanding electronic [1,2], mechanical [3] and thermal properties [4]. Unlike graphene by zero energy gap, few-layer BP possesses a direct energy gap in the electronic band. BP shows great advances on the high room-temperature transporting electron mobility, ~1000 cm<sup>2</sup>V<sup>-1</sup>s<sup>-1</sup> and large on/off current ratio in BP-based electronic device [1,2]. The intrinsic atomic structure of BP leads to interesting anisotropic mechanical and thermal properties as well as negative Poisson ratio [3]. Therefore, BP holds great promise for various applications in 2D

\*\* Corresponding author.

semiconductor devices.

However, BP is chemically unstable in air [5,6]. In ambient environment the phosphorous atoms of BP can react with oxygen and water easily. To prevent such chemical reaction or isolate BP from oxygen and water, the most convenient and efficient method is wrapping/covering BP by other more environment-inert materials, such as graphene (Gr), boron nitride (BN) and dielectric/fluoropolymer [7,8]. In particular, graphene, which has high thermal conductivity [9–11], larger surface area and mechanical properties, is considered as the best coverage [12]. For instance, the metal templates (such as Cu, Ni and Ru) can be protected from oxidation by depositing graphene on them [13,14]. The long-term stability of BP covered by graphene in air exposure has been reported by Kim et al. [6]. Their experimental results show that graphene can be used as a passivation layer to protect BP from chemical reaction in ambient environments. When BP is covered by few-layer graphene, thermal transport through the BP/Gr interface is the major route for heat dissipation. The BP/Gr interfacial layers are coupled by the



<sup>\*</sup> Corresponding author.

*E-mail addresses*: junhua.zhao@163.com (J. Zhao), nwei@nwsuaf.edu.cn (N. Wei).

weak van de Waals (vdWs) interactions and thus low thermal conductance is expected. Since thermal conductivity limits the maximum current density, the poor thermal performance of a heterogeneous structure limits its application in Micro/Nano-Electro-Mechanical Systems [15]. The accumulated Joule heat nucleates thermal hot spots, and potentially causes failure of devices. Therefore, it is of great significance to improve the performance of interfacial thermal conductance (ITC) becomes an urgent need. Although thermal properties of BP, along both in-plane and cross-plane directions, have been well studied [16–19], their ITC with dissimilar materials, such as graphene have not been investigated systematically.

To improve the ITC, many approaches with various techniques were developed by enhancing interfacial interaction or/and reducing the phonon spectra mismatch at the interface. For example, Gao and Müller-Plathe [20] reported that the ITC of graphene-polyamide-6,6 nanocomposites by surface-grafted polymer chains is improved remarkably and their ITCs increase continuously with the surface density of grafted chains. Lin and Buehler [21] found that the alkyl-pyrene molecules, which possess phonon-spectra features of both graphene and octane, can act as phonon-spectra linkers to bridge the vibrational mismatch at the graphene/octane interface. The advantage of this approach is that the non-covalent functionalization does not induce additional defects or adatoms in graphene. It also enhances the thermal performance of nanocomposites while retaining the intrinsic mechanical and thermal properties of pristine graphene. Liu Ling and co-workers [22] reported that the thermal conductance across the interfaces between graphene and polymethyl methacrylate (PMMA) can be improved around 273% by introducing hydrogenbond-capable hydroxyl groups to the interfaces. The coupling of the low-frequency vibration modes is enhanced. The improvement of the ITC is mainly attributed to the strengthening of the interfacial interactions. The energy between hydrogen bond interactions is around 1-2 orders of magnitude stronger than that of vdWs interactions. Furthermore, Ding et al. [23] reported that the presence of defects in the interface can increase the interfacial friction and excite more shear modes of phonon. Consequently, the thermal conductance is enhanced considerably.

Herein we studied ITC of a BP/Gr heterostructures using both non-equilibrium molecular dynamics (NEMD) and thermal relaxation methods. Each method has its own advantages. The NEMD simulation provides steady state phonon transport information and is helpful in understanding the thermal conductivity of the overall heterostructures. The thermal relaxation method mimics experimental laser-based pump-probe process and is used to measure ITC. By using this approach, two important parameters are identified. One is the critical heat power density per area, P<sub>cr</sub>, which could maintain the thermal stability of the system, and the other is the maximum heat power density per area  $P_{max}$ , which can be loaded in the system. We also manipulate the interfacial thermal conductance by altering cross-plane compressive strain and interface defect engineering. The relationship between the interfacial thermal conductance and the phonon spectra at the interface is discussed in great details. Our work suggests that the interfacial thermal conductance can be effectively tuned in a wide range for different external strain and interfacial defects.

#### 2. Modeling and methodology

To build and minimize the lattice mismatch of the heterostructure of BP and graphene, the supercell of BP sheet with  $6 \times 19$ unit cells is chosen (with armchair edge along the *x*-direction, see Fig. 1(a)). The graphene supercell is made of  $15 \times 11$  unit cells (with zigzag edge along the *x*-direction see Fig. 1(b)). Thus there exits small mismatch between BP and graphene in *x* and *y* directions (1.56% and 0.054%), respectively. Based on the supercells of graphene and BP, BP/Gr heterostructures are created with the cross-section area about 2.67 nm  $\times$  6.30 nm (as shown in Fig. 2(a–c)).

All molecular dynamics (MD) simulations are performed using the large-scale atomic/molecular massively parallel simulator (LAMMPS) package [24]. The Stillinger-Weber (SW) potential [25] is employed to describe the covalent interaction between phosphorous atoms, while the interactions of carbon atoms in multilayer graphene are described by AIREBO potential [26]. The van der Waals interactions of interlayers are modeled with 12-6 Lennard-Jones (LJ) potential and the corresponding parameters are listed in Table 1 [27]. The cutoff distance of the LJ potential is set as 1.2 nm. A time step of 0.5 fs is employed in the MD simulations. Two simulation models, periodic (Fig. 2(a)) and non-periodic (Fig. 2(c)) boundary conditions in thermal transport directions, are employed to explore the ITC at BP/Gr interface using direct NEMD and thermal relaxation methods, respectively.

#### 2.1. NEMD-periodic method

To calculate ITC based on the reverse NEMD or MP method [28], the periodic boundary condition model (Fig. 2(a)) is employed. In this model, periodic boundary conditions are applied in all the three dimensions. The initial configuration is firstly equilibrated at NPT ensemble (constant temperature and pressure) with room temperature at 300 K and pressure at 1 bar for 0.5 ns ( $1 \times 10^{6}$  time steps) to optimize the structure of system. Afterwards, the system is then switched to be at the microcanonical ensemble (NVE). The ITC between BP and graphene layers is investigated by MP approach. The system is equally divided into 40 slabs along the heat transport direction (z-dimension), with the heat source and heat sink selected in the middle and at the ends of the model, respectively (see Fig. 2(a and b)). The heat flux is added by exchanging the kinetic energies between the hottest atom in the heat sink slab and the coldest atom in the heat source slab, the heat flux can be obtained by:

$$J = \frac{\sum_{Nswap^{\frac{1}{2}}} \left( mv_h^2 - mv_c^2 \right)}{t_{swap}},\tag{1}$$

where  $N_{swap}$  and  $t_{swap}$  are the entire swap time and number of swaps, The  $t_{swap}$  is the time scale to perform kinetic energy exchange every  $t_{swap}$ . The larger value of  $t_{swap}$  suggests lower exchange frequency and induces lower  $\Delta T$  at the interface, while,  $v_h$ and  $v_c$  are the atomic velocities of the hottest and coldest atoms, respectively. To ensure that the system can reach the nonequilibrium steady state before data collecting, we monitor the temperature of each layer with time (Fig. S1 in supporting information (SI)). The temperature *T* refers to the average temperature of all atoms in each layer

$$T_i(slab) = \frac{2}{3Nk_B} \sum_j \frac{p_j^2}{2m}.$$
 (2)

Our results show that the system reaches a non-equilibrium state after 2.0 ns. The temperature distribution is obtained by calculating the average data over the following 3 ns, as shown in Fig. 3 (a). The thermal conductance *G* is calculated using  $G = J/(2 \times \Delta T \times A)$ , where *A* is the cross-section area and  $\Delta T$  is the temperature difference at the interface and the factor 2 is due to the fact that the heat current propages in two directions. The time-averaged temperature profile, illustrated in Fig. S2 (see SI), shows that there is greater temperature jump  $\Delta T$  at the interface close to

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