Electron-phonon coupling in a honeycomb borophene grown on Al(111) surface

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In this paper, we explore the possible superconductivity in h-B2 grown on an Al(111) substrate. (Dated: February 19, 2019)

I. INTRODUCTION

Boron possesses rich chemistry like carbon. Since the discovery of graphene, great effort has been made to synthesize two-dimensional (2D) boron sheet, namely borophene. In sharp contrast to graphene, it was suggested from theoretical calculations that a borophene favors a triangular lattice structure with a special vacancy order, exemplified by the so-called α- or β-sheet structured borophene [1,2]. Recently, three different structured borophene were successfully grown on Ag(111) surface by direct evaporation of boron atoms [3,4]. One has a buckled structure (b-B3) without vacancies, while the other two have vacancy orders, named as β12-B5 and χ3-B4, respectively.

Searching for superconductivity in 2D compounds is of great interest, because it has potential application in constructing nano-scale superconducting devices with single-electron sensitivity [5,6]. In addition to graphene and borophene, phosphorene [7,8], silicene [9,10], germanene [11,12], and stanene [13,14] have all been synthesized in laboratory. Phosphorene is a semiconductor with a direct bandgap of 1.51 eV [15]. Silicene, germanene, and stanene are zero-gap semimetals with vanished density of states at the Fermi energy [16,17], similar to graphene. As a result, additional charge doping must be introduced to induce superconductivity. In recent years, a number of theoretical calculations have been done to explore the possibility of superconductivity with high transition temperature in these doped 2D materials [18-25]. More specifically, a superconducting transition was predicted to occur at a temperature as high as 31.6 K in heavily electron-doped phosphorene [25]. Similar prediction was made for arsenene [26]. However, superconductivity was only observed in Li-intercalated few-layer graphene at 7.4 K [27], in magic-angle graphene superlattice at 1.7 K [28], and in bilayer stanene below 1 K [29]. This suggests that it is difficult to dope charge into these systems up to the level assumed in theoretical calculations.

Different from these zero-gap or gapped 2D compounds, borophenes, including h-B2, β12-B5, χ3-B4, are all intrinsic metals [3,4]. They are good candidates of intrinsic 2D superconductors. From first-principles electronic structure calculations for the electron-phonon coupling (EPC), it was predicted that these three free-standing borophenes could become superconducting around 20 K even without doping [30-33]. However, the tensile strain with the electron transfer imposed by the Ag substrate can significantly suppress the superconducting transition temperature $T_c$. For example, the $T_c$ of β12-B5 could be dramatically reduced to 0.09 K by a biaxial tensile strain of 2% with an electron transfer of 0.1 e/boron [34]. Thus, it is indispensable to include the substrate effect in the calculation of EPC in borophenes and other 2D materials.

Recently, a honeycomb borophene (h-B2) was successfully grown on the Al(111) substrate (abbreviated as h-B2/Al(111) hereafter) [35]. From first-principles electronic structure calculations, it was found that the honeycomb structure is stabilized by a significant charge transfer from Al(111) to h-B2 [35]. Similar as in MgB2 whose honeycomb boron sheet plays a central role in pairing electrons in a relatively high $T_c$ [36], a free-standing h-B2 was also predicted to be a 30 K superconductor by ignoring the imaginary phonon modes [31]. However, it is not clear whether such high-$T_c$ superconductivity can survive in h-B2 grown on an Al(111) substrate.

In this paper, we explore the possible superconductivity in h-B2/Al(111) by calculating its electronic structure, lattice dynamics, and EPC using the first-principles density functional theory and the Wannier interpolation technique. The influ-
ence of the Al substrate is fully considered in our calculations, which allows both the charge transfer and strain effects to be more precisely determined. After full optimization, we find that h-B$_2$/Al(111) has a buckling lattice structure with a tiny buckling height of 0.035 Å. The $sp^2$-hybridized $\sigma$-bonding bands of h-B$_2$/Al(111) are partially filled, but the intra-boron-layer EPC in this material is weak due to the hardening of phonons and the reduced phonon DOS. However, there is a strong coupling between Al phonons and electrons in h-B$_2$. Based on this property, we propose a monolayer AlB$_2$ material with an EPC constant $\lambda$ about 35% larger than in MgB$_2$ \cite{37}. Using the McMillian-Allen-Dynes formula, we predict that the superconducting $T_c$ of this monolayer AlB$_2$ is about 6.5 K.

II. COMPUTATIONAL METHOD

In the calculations, the plane wave basis method was adopted \cite{38}. We calculated the Bloch states and the phonon perturbation potentials \cite{39} using the local density approximation and the norm-conserving pseudopotentials. The kinetic energy cut-off and the charge density cut-off were taken to be 80 Ry and 320 Ry, respectively. The charge densities were calculated on an unshifted mesh of 40×40×1 points in combination with a Methfessel-Paxton smearing \cite{40} of 0.02 Ry. The dynamical matrices and the perturbation potentials were calculated on a $\Gamma$-centered 10×10×1 mesh, within the framework of density-functional perturbation theory \cite{41}.

To avoid the influence of Al surface states on a fracture surface, we employed a slab model with inversion symmetry to simulate h-B$_2$/Al(111) [Fig. 1]. There are seven Al layers with one h-B$_2$ on each surface. The thickness of vacuum layer in the slab was set to 8.58 Å. The experimental value of the in-plane lattice constant of the Al(111) surface, 2.8635 Å \cite{42}, was adopted. Al atoms in the middle three layers were fixed to mimic the bulk, the other Al layers and two h-B$_2$ sheets were relaxed to minimize the total energy.

The maximally localized Wannier functions (MLWFs) \cite{43,44} were constructed on a 10×10×1 grid of the Brillouin zone. We used 38 Wannier functions to describe the band structure of h-B$_2$/Al(111) around the Fermi level. Among them, four are $p_z$-like states associated with the boron atoms, six are $\sigma$-like states localized in the middle of boron-boron bonds, the other 28 functions correspond to the $\sigma$ states localized in the middle of boron-boron bonds, respectively. For instance, the average spatial spread of the six $\sigma$-like states is just about 1.01 Å$^2$. Fine electron (360×360×1) and phonon (120×120×1) grids were used to interpolate the EPC constant through the Wannier90 and EPW codes \cite{43,45}. The Dirac $\delta$-functions for electrons and phonons were smeared out by a Gaussian function with the widths of 50 meV and 0.2 meV, respectively.

The EPC constant $\lambda$ was determined by the summation of the momentum-dependent coupling constant $\lambda_{\mathbf{q} \nu}$ or $\lambda_{\mathbf{k} m}$ over the first Brillouin zone, or the integration of the Eliashberg spectral function $\alpha^2 F(\omega)$ \cite{37,38}.

$$\lambda = \frac{1}{N_q} \sum_{\mathbf{q} \nu} \lambda_{\mathbf{q} \nu} = \frac{1}{N_k} \sum_{\mathbf{k} m} \lambda_{\mathbf{k} m} = 2 \int \frac{\alpha^2 F(\omega)}{\omega} d\omega, \quad (1)$$

where $N_q$ and $N_k$ represent the total numbers of $\mathbf{q}$ and $\mathbf{k}$ points in the fine $\mathbf{q}$-mesh and $\mathbf{k}$-mesh, respectively. The coupling constant $\lambda_{\mathbf{q} \nu}$ and $\lambda_{\mathbf{k} m}$ read

$$\lambda_{\mathbf{q} \nu} = \frac{2}{\hbar N(0) N_k} \sum_{n \mathbf{q} \nu \mathbf{q} \nu} |g_{\mathbf{k} \mathbf{q} \nu}^{(m)}|^2 \delta(\epsilon_{\mathbf{k}}^{(n)}) \delta(\epsilon_{\mathbf{k} + \mathbf{q}}^{(m)}), \quad (2)$$

and

$$\lambda_{\mathbf{k} m} = \frac{2}{\hbar N(0) N_q} \sum_{\nu \mathbf{q} \nu \mathbf{q} \nu} |g_{\mathbf{k} \mathbf{q} \nu}^{(m)}|^2 \delta(\epsilon_{\mathbf{k}}^{(n)}) \delta(\epsilon_{\mathbf{k} + \mathbf{q}}^{(m)}), \quad (3)$$

The Eliashberg spectral function $\alpha^2 F(\omega)$ was calculated with

$$\alpha^2 F(\omega) = \frac{1}{\hbar N(0) N_q N_k} \sum_{\nu \mathbf{q} \nu \mathbf{q} \nu} |g_{\mathbf{k} \mathbf{q} \nu}^{(m)}|^2 \delta(\epsilon_{\mathbf{k}}^{(n)}) \delta(\epsilon_{\mathbf{k} + \mathbf{q}}^{(m)}) (\omega - \omega_{\mathbf{q} \nu}). \quad (4)$$

Here $\omega_{\mathbf{q} \nu}$ is the phonon frequency and $g_{\mathbf{k} \mathbf{q} \nu}^{(m)}$ is the probability amplitude for scattering an electron with a transfer of crystal momentum $\mathbf{q}$, $n$, $m$ denote the indices of energy bands and phonon mode, respectively. $\epsilon_{\mathbf{k}}^{(n)}$ and $\epsilon_{\mathbf{k} + \mathbf{q}}^{(m)}$ are the eigenvalues of the Kohn-Sham orbitals with respect to the Fermi level. $N(0)$ is the density of states (DOS) of electrons at the Fermi level. From $\lambda_{\mathbf{q} \nu}$ or $\lambda_{\mathbf{k} m}$, we can identify which phonon mode or electronic state has larger contribution to the EPC.

The superconducting transition temperature is determined by the McMillian-Allen-Dynes formula \cite{48},

$$T_c = \frac{\omega_{\mathbf{q} \nu}}{1.2} \exp \left[ \frac{-1.04(1 + \lambda)}{\lambda(1 - 0.62 \mu^*) - \mu^*} \right]. \quad (5)$$

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig1.png}
\caption{Slab model of h-B$_2$/Al(111). (a) Top view plotted with the depth-cueing technique. (b) Side view. The green and slate balls represent boron and Al atoms, respectively. The thick black line denotes the unit cell.}
\end{figure}
we find that in h-B$_2$/Al(111). By calculating the Bader charge decomposition [50, 51], the outward boron atom is 1.15 (0.87) e mainly by the outmost Al atom. While in the bulk AlB$_2$ bands crossing the Fermi level. By projecting λ boron atom acquires about 1.46 electrons.

The outmost Al layer are 13.61 Å and 1.39 Å, respectively. Al substrate and the average distance of boron atoms from of the triangular lattice of outmost Al layer [Fig. 1(a)], is energetic favored. After optimization, the total thickness of Al substrate and the average distance of boron atoms from the outmost Al layer are 13.61 Å and 1.39 Å, respectively. The h-B$_2$ layer is nearly flat with a tiny buckling of 0.035 Å, not reported in the previous calculation [35]. This buckling structure is robust. It exists even when the vacuum layer is increased to 23.58 Å.

From the calculation, we find that the crystal structure of h-B$_2$/Al(111), with boron atoms occupying the hollow sites of the triangular lattice of outmost Al layer [Fig. 1(a)], is energetically favored. After optimization, the total thickness of Al substrate and the average distance of boron atoms from the outmost Al layer are 13.61 Å and 1.39 Å, respectively. The h-B$_2$ layer is nearly flat with a tiny buckling of 0.035 Å, not reported in the previous calculation [35]. This buckling structure is robust. It exists even when the vacuum layer is increased to 23.58 Å.

FIG. 3. Fermi surfaces formed by the nine bands across the Fermi level in h-B$_2$/Al(111) in the reciprocal unit cell. Different colors represent the strength of $\lambda_{10}$. We label these nine Fermi surfaces as FS-$\alpha$, with $\alpha$ running from $a$ to $i$.

FIG. 2. Band structures of h-B$_2$/Al(111). The width of red lines is proportional to the contribution of the $sp^2$-hybridized $\sigma$-bonding orbitals to the Kohn-Sham states. The blue circles are obtained by interpolation of MLWFs. The Fermi level is set to zero.

III. RESULTS AND ANALYSIS

Figure 2 shows the band structures of h-B$_2$/Al(111). There are nine bands across the Fermi level. The MLWFs interpolated band structure agrees excellently with the first-principles calculation. This, together with the high locality of MLWFs, sets a solid foundation for accurately computing the EPC using the Wannier interpolation technique. The orbital-resolved band structure suggests that the B-B $sp^2$-hybridized $\sigma$-bonding bands are partially occupied, similar as in MgB$_2$, but the $\sigma$-bonding bands in the bulk AlB$_2$ are completely filled [49]. By calculating the Bader charge decomposition [50, 51], we find that in h-B$_2$/Al(111), the charge transfer to the inward (outward) boron atom is 1.15 (0.87) e/boron, contributed mainly by the outmost Al atom. While in the bulk AlB$_2$, each boron atom acquires about 1.46 electrons.

Figure 3 shows the Fermi-surface contours for the nine bands crossing the Fermi level. By projecting $\lambda_{10}$ onto these Fermi surfaces, we find that electrons on the Fermi surfaces around the $\Gamma$ (Fig. 3(a)-Fig. 3(d)) and $M$ (Fig. 3(h)) points couple strongly with phonons. From Fig. 2 we know that the $\Gamma$-centered Fermi sheets stem from the $sp^2$-hybridized B-B $\sigma$-bonding bands. The orbitals of B-$p_z$ and Al comprise the electronic states around the $M$ point on FS-$h$. Compared with the outward boron atoms, there are more electrons transferred to the inward ones, causing the $p_z$ orbitals more insulating, especially around the $M$ point.

Figure 3 shows the lattice dynamics of h-B$_2$/Al(111). A gap of about 10 meV is found in the phonon spectrum [Fig. 3(a)]. Due to the large difference between the masses of boron and Al atoms, it is straightforward to assign the modes above and below the gap mainly to boron and Al atoms, respectively. This assumption is confirmed by the result of projected phonon DOS calculated under the quasi-harmonic approximation [Fig. 3(b)]. The phonons at the $\Gamma$ point have the largest coupling with electrons. The strongly coupled modes of h-B$_2$ at the $\Gamma$ point are identified to be $A_{2g}$, $A_{1g}$, $E_u$, and $E_g$ [Fig. 4(a)]. The phonon DOS attributed to boron atoms can be classified into two regions [Fig. 3(c)]. From 50 meV to 70 meV, the phonons originate from the out-of-plane movements of boron atoms. The in-plane displacements of boron atoms mainly participate in the phonons above 100 meV. This indicates that the strongly coupled $E_u$ and $E_g$ modes at about 104 meV are mainly the contribution of the in-plane bond-stretching phonon modes.

The vibrational patterns of strongly coupled phonons at the $\Gamma$ point above the frequency gap are schematically shown in Fig. 3. The amplitudes of Al displacements in the strongly coupled phonon modes gradually decrease with the increase of vibrational frequency. This agrees with the fact that the frequencies of the Al phonon modes lie mainly below 40 meV. Particularly, the high-frequency $E_u$ and $E_g$ phonons only involve the 2D bond-stretching motions of boron atoms.
three regions separated by two gaps [Fig. 6(a)]. A large proportion of the phonons are strongly coupled at Γ. The mode symmetries of strongly coupled phonon modes at Γ are labelled on the right side. (b) Projected phonon density of states. (c) Decomposed boron-related phonon density of states along three directions.

FIG. 4. Lattice dynamics of h-B₂/Al(111). (a) Phonon spectrum with a color representation of \( \lambda_{\nu} \) at a given wave vector and mode. The mode symmetries of strongly coupled phonon modes at Γ are labelled on the right side. (b) Projected phonon density of states. (c) Decomposed boron-related phonon density of states along three directions.

FIG. 5. Vibrational patterns for strongly coupled phonon modes of h-B₂ at the Γ point. The red arrows and their lengths denote the directions and relative amplitudes of atomic movements, respectively.

The Eliashberg spectral function \( \alpha^2 F(\omega) \) is divided into three regions separated by two gaps [Fig. 5(a)]. A large proportion of \( \alpha^2 F(\omega) \) lies below 40 meV. This indicates that the Al-associated phonons play a vital role in the EPC of h-B₂/Al(111). With respect to \( F(\omega) \) [Fig. 5(b)], the sharp peaks of \( \alpha^2 F(\omega) \) around 55 meV and 104 meV show that there exist strongly coupled B-associated phonons, such as the \( A_{2u}, A_{1g}, E_{\sigma}, \) and \( E_{\pi} \) modes [Fig. 5]. The EPC constant \( \lambda \) and \( \omega_{\text{ph}} \) are found to be 0.64 and 22.15 meV. The Al-associated and B-associated phonons contribute 76.6% and 23.4% to the total \( \lambda \), respectively. We also find that there is a strong interfacial coupling between Al phonons and electrons in h-B₂. It occupies about 30.7% of the total \( \lambda \).

IV. DISCUSSION

The Eliashberg formula was established for a superconductor with translational symmetry. Attention, however, should be paid in the calculation of EPC in 2D compounds using this formula when a metallic substrate is included. In particular, Al is a good metal with a large bandwidth. More Al-associated electronic bands would appear around the Fermi level if the thickness of Al substrate gradually increases in the slab model that we used to simulate h-B₂/Al(111). The contribution of h-B₂ to the EPC will be submerged by the significant reduction of boron atoms to the DOS around the Fermi level. As a result, the EPC of h-B₂/Al(111) supercell will approach to the EPC of bulk face-centered-cubic (fcc) Al [52], when the substrate becomes semi-infinite in the slab model. Thus the intrinsic EPC of h-B₂ need to be extracted reasonably from current data. Moreover, the previously obtained \( \lambda \) (0.64) and \( \omega_{\text{ph}} \) (22.15 meV) can not be substituted directly into the McMillan-Allen-Dynes formula to determine the \( T_c \) of h-B₂/Al(111).

Since the boron and Al phonon vibrations are well separated in frequency, we can regard the EPC generated by boron phonons as the EPC of h-B₂ if the interfacial coupling between the boron phonons and the electronic states from the substrate can be properly deduced. We calculated \( \lambda_{\text{nn}} \) in the frequency region from 50 to 140 meV. It is found that the \( \sigma \)-bonding electrons of h-B₂ contribute 39.1% (62.6%) to the EPC caused by the out-of-plane (in-plane) boron phonons. So the \( \alpha^2 F(\omega) \) in the intervals [50, 100] meV and [100, 140] meV should be reduced by 60.9% and 37.4%, respectively, if we assume \( \alpha^2 F(\omega) \) depends weakly on \( \omega \). Furthermore, the EPC constant can not be normalized by the whole DOS of the h-B₂/Al(111) supercell at the Fermi level [see Eq. (2)]. Instead, it should be normalized only by the electron DOS of h-B₂. At the Fermi level, the total DOS and the DOS contributed by the h-B₂ electrons are 1.91 and 0.62 states/spin/eV/cell, respectively. From the refined \( \alpha^2 F(\omega) \) of h-B₂, which is shown in Fig. 6(b), we find the value of \( \lambda \) for h-B₂ is only 0.23.

The usage of inversion slab with two h-B₂ sheets may raise the question about the double counting. The validity of our calculations lies in the fact that these two h-B₂ sheets will be decoupled when the substrate is sufficiently thick. The appearance of both the doubly degenerate \( \sigma \)-bonding bands and the nearly doubly degenerate boron phonon modes indicates that the interaction between these two h-B₂ sheets is extremely weak. To further justify the decoupling assumption made in our current slab model, we also calculated the band structure and phonon spectrum for a thicker slab with 19 Al layers and two h-B₂ sheets. After relaxation, the substrate is as thick as 40.65 Å. We find that the \( \sigma \)-bonding bands of h-B₂ are entirely unchanged. For strongly coupled phonons modes at the Γ point, the frequency of \( E_{\pi} \) modes has the largest relative deviation, whose value is only about 0.11% in comparison to the result of the current slab model. Hence, the coupling between these two h-B₂ sheets in current slab model can be ignored.
The EPC of h-B$_2$ behaves differently from that in MgB$_2$, although the metallic $\sigma$-bonding bands of h-B$_2$ are preserved in h-B$_2$/Al(111). At the $\Gamma$ point, detailed analysis shows that the EPC matrix elements of the bond-stretching modes ($E_u$ and $E_g$) in h-B$_2$ are indeed comparable to those of $E_{2g}$ modes in MgB$_2$. However, the phonon DOS per h-B$_2$ near the $E_g$ modes is compressed with respect to that around the $E_{2g}$ modes in MgB$_2$, due to well-separated out-of-plane and in-plane boron phonons [Fig. 4(c)]. Moreover, the frequencies of $E_u$ and $E_g$ modes at the $\Gamma$ point are higher than the $E_{2g}$ mode in MgB$_2$ (70.8 meV) [53]. These two effects reduce the EPC in h-B$_2$.

Motivated by the existence of a strong coupling between boron and Al atoms, we calculated the EPC in a monolayer structured AlB$_2$, including a h-B$_2$ and a single Al layer. Figure 4(c) shows the calculated spectrum of $\alpha^2 F(\omega)$. In comparison with h-B$_2$/Al(111), the peak of $\alpha^2 F(\omega)$ arises from the Al phonons shifts from 35 meV to a lower frequency in this monolayer AlB$_2$. The high-frequency peaks of $\alpha^2 F(\omega)$ in monolayer AlB$_2$ are also red-shifted, because the lattice constant for monolayer AlB$_2$ is 2.5% larger than that of h-B$_2$/Al(111). As a consequence, a dramatic enhancement in $\lambda$ (1.01) and a reduction in $\omega_{\text{log}}$ (17.82 meV) are obtained.

The Coulomb pseudopotential $\mu^*$ is commonly used as a free parameter to fit experimental $T_c$. To predict the $T_c$ for the monolayer AlB$_2$ more accurately, we deduce the value of $\mu^*$ from the bulk AlB$_2$. The spectrum of $\alpha^2 F(\omega)$ for the bulk AlB$_2$ generated by Wannier interpolation is shown in Fig. 4(d), consistent with the result presented in Ref. [53]. $\alpha$ and $\omega_{\text{log}}$ for AlB$_2$ are estimated to be 0.46 and 45.30 meV, respectively. There would be no superconductivity in the bulk AlB$_2$ if $\mu^*$ is set to 0.23. Assuming this is also the value of $\mu^*$, we find the $T_c$ of the monolayer AlB$_2$ will be about 6.5 K.

Compared with bulk AlB$_2$, the superconductivity in monolayer AlB$_2$ is closely related to the distance $(h_{\text{Al-B}})$ between Al and honeycomb boron sheet, with $h_{\text{Al-B}}=1.37$ Å in monolayer AlB$_2$, and 1.63 Å in bulk AlB$_2$ [54]. The correlation between $T_c$ and such distance also exists in graphite intercalated compounds. For instance, $h_{\text{Ba-C}}=2.62$ Å, $h_{\text{Sr-C}}=2.47$ Å, and $h_{\text{Ca-C}}=2.26$ Å [55] in nonsuperconducting BaC$_6$, SrC$_6$ ($T_c=1.65$ K) [56], and CaC$_6$ ($T_c=11.5$ K) [57, 58], respectively. Now, monolayer AlB$_2$ and fcc Al are two superconductors, with $T_c$ being 6.5 K and 1.2 K, respectively. If we splice these two compounds together along the [111] direction of fcc Al, the structure of h-B$_2$/Al(111) will reappear exactly. In that sense, analogous superconductivity in h-B$_2$/Al(111) can be anticipated in experiment, as in monolayer AlB$_2$.

V. SUMMARY

Based on the first-principles density functional theory and the state-of-the-art Wannier interpolation technique, we calculate the EPC for h-B$_2$ grown on an Al(111) substrate. We simulate the substrate effect using a slab model. Similar as in MgB$_2$, we find that the $\sigma$-bonding bands are also metallized in h-B$_2$/Al(111). However, the EPC constant $\lambda$ in h-B$_2$ is significantly smaller than in MgB$_2$, due to the blue shift of the bond-stretching boron phonons and the reduction of phonon DOS. Furthermore, we find that the interlayer coupling between Al-associated phonons and electrons on the h-B$_2$ is quite strong. Based on this observation, we predict that a borophene decorated by just one Al layer, i.e., monolayer AlB$_2$, could become a superconductor below 6.5 K. We also suggest that similar superconducting $T_c$ can be detected in h-B$_2$/Al(111).

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