Investigation of Moiré Phonon Systems in Twisted *h*-BN Structure

Sabin Park[1] and Lukas P. A. Krisna[2]

[1] *Department of Materials Engineering, School of Engineering, The University of Tokyo*

[2] *Department of Physics, Graduate School of Science, Osaka University*

This report explores the implications of moiré superlattices on phonon systems within two-dimensional materials, particularly through a graphene/twisted hexagonal boron nitride (*h*-BN) structure to detect phonon-related optical properties in twisted *h*-BN.

Authors

Sabin Park is engaged in the study of electromagnetic properties of graphene and other two-dimensional materials in the infrared regime. In this research, he was responsible for device fabrication and optical measurement.

Lukas P. A. Krisna: is engaged in the calculation of electronic and phononic band structures in moiré systems of two-dimensional materials. In this research, he was responsible for theoretical predictions of material properties.

Introduction and Background

Moiré superlattices have attracted significant interest for their unique effects on electronic and phonon properties in two-dimensional materials like graphene and transition metal dichalcogenides (TMDs). While considerable attention has been given to their electronic properties [1-3], the impact on phonons remains less explored[4]. Recent theoretical advancements suggest that moiré effects on phonon systems could open new research avenues. We recently became interested in moiré phonons in *h*-BN, illustrated in Figure 1(a). We have the device fabrication skills and experimental setups to observe those phenomena. However, as it is a new area of research, we need to establish theoretical foundations to support our experimental findings. To address it, we decided to collaborate with Lukas, a specialist in theoretical calculations from Prof. Koshino's group, which is a pioneer in the study of phonons in moiré systems[5]. Figure 1(b) shows a calculated phonon band structure of the

Graphene/*h*-BN moiré system with atmoic reconstruction studied by Lukas[6]. Collaborating with Lukas, we initiated this study to explore these uncharted territories using twisted *h*-BN, hypothesizing it as an ideal system for observing moiré-induced phenomena related to phonons.

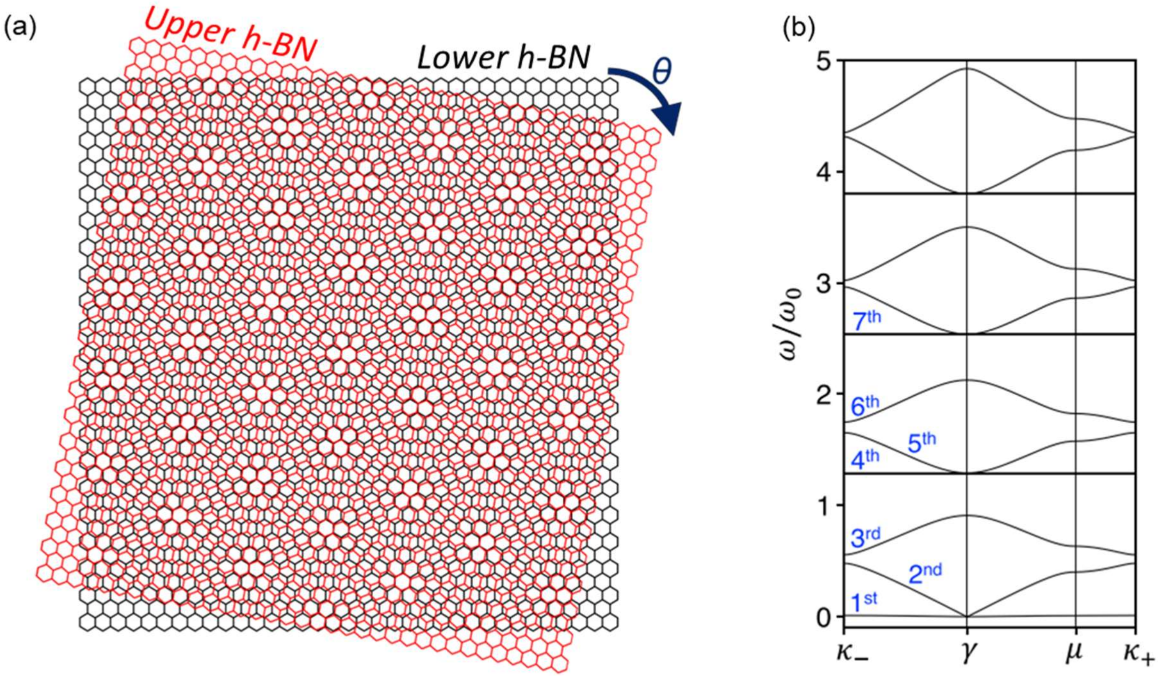

Figure 1: (a) Schematic illustration for *h*-BN/*h*-BN system with the twist angle. (b) Phonon dispersion of limiting case in graphene/*h*-BN moiré structure with atomic reconstruction.

Methodology and Results

Our experimental approach involves using a graphene/twisted *h*-BN structure to detect phonon-related optical properties through photo-thermoelectric measurements. It has been reported that *h*-BN reflects incident light near 7.3-μm wavelength due to optical phonon modes[7-9]. Inspired by this report, Lukas hypothesized that there could be unexplored light-matter interactions involving moiré-modified optical phonons, which vary depending on twist angle of *h*-BN layers. Initially, we confirmed the reflection of light by phonons in *h*-BN near 7.3-μm wavelength through the decline of the photovoltage (V_{ph}) using an existing *h*-BN/graphene/*h*-BN/Graphite device. Figure 2(a) shows a schematic illustration of the device structure. Figure 2(b) shows in-plane *n* and *k* of *h*-BN with respect to wavelength of photons, where *n* and *k* denote real part and imaginary part of the complex refractive index. The graph shows a distinct peak at 7.3 μm, which can be attributed to the transverse optical (TO) phonons. This peak indicates the presence of the Reststrahlen band of the optical phonon. Figure 2(c) presents the measurement data of the amplitude of photovoltage $|V_{ph}|$ as a function of the wavelength of the irradiation. $|V_{ph}|$ exhibited its significant decline, dropping to ~0.56 μV at 7.3-μm wavelength. The detail of our optical measurement system is displayed in Figures 3(a-c).

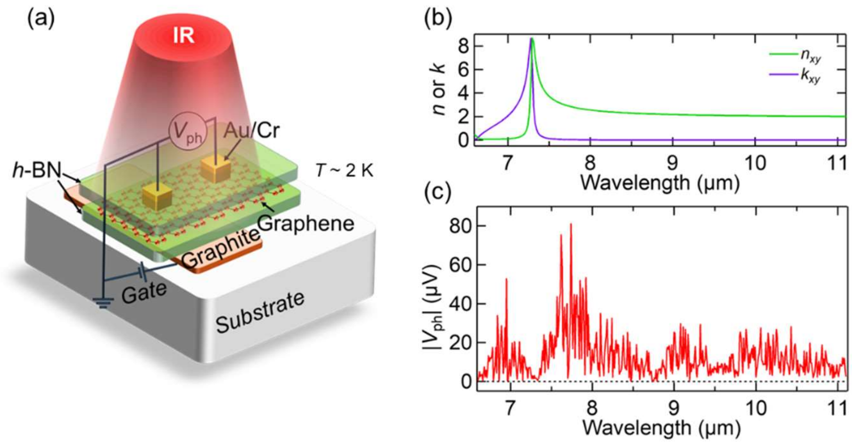

Figure 2: (a) Schematic of the device structure with IR radiation. (b) In-plane *n* and *k* of *h*-BN with respect to the wavelength of photon. (c) Experimental data of $|V_{ph}|$ versus wavelength. Dip at 7.3 μm indicates Reststrahlen band of *h*-BN.

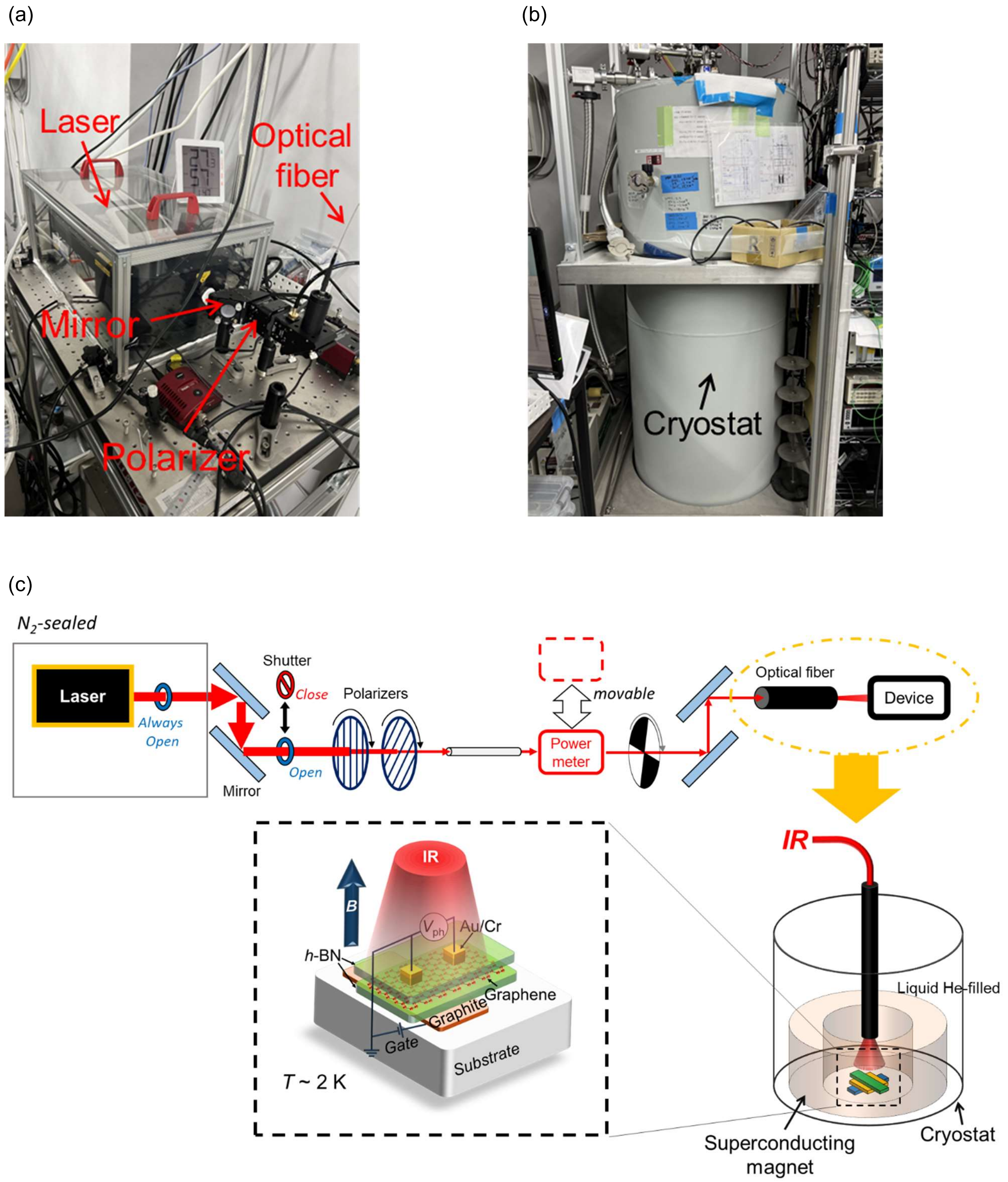

Figure 3: Optical measurement system: (a) A laser, mirrors, polarizers, an optical fiber; (b) A cryostat. (c) Schematic illustration of the system.

Furthermore, we fabricated graphene/h-BN structure device that exploits parallel-stacked ($\theta = 0°$) bilayer h-BN to confirm our fabrication skills for twisted h-BN. We used the tear-and-stack method to make bilayer h-BN, carefully adjusting the twist angle to optimize moiré configurations. Figures 4(a-d) show each layer composing the device. After we fabricated the stacked structure on SiO_2/Si substrate, we made electrodes through electron beam lithography, reactive ion etching, and electron beam evaporation. Figure 4(e) shows an optical micrograph of the device with metal electrodes. Figure 4(f) shows the schematic of the device structure with Au/Cr electrodes. Electrode patterns are defined by electron beam lithography. The top h-BN was selectively etched along to the pattern, leaving the graphene underneath. Au and Cr are deposited to the selectively etched top h-BN by electron beam evaporation. The device will be measured after mesa etching.

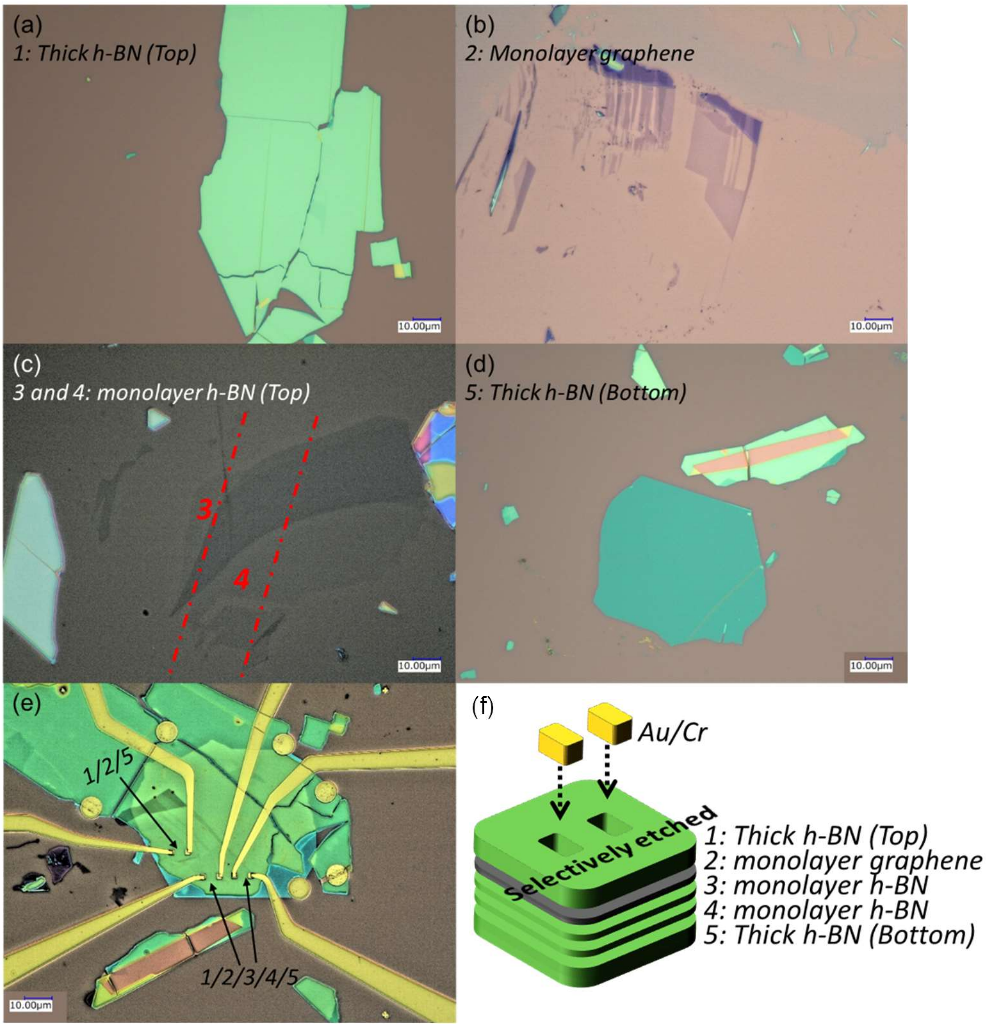

Figure 4: (a-d) Optical micrographs of each layer. (e) Optical micrograph of the stacked structure with electrodes. (f) Schematic of the device

Conclusion and Future Work

After measuring the parallel-stacked bilayer *h*-BN device and evaluating its quality, we plan to fabricate graphene/twisted *h*-BN devices to explore light-matter interaction of involving moiré-modified optical phonons in twisted *h*-BN. Through forthcoming measurements and theoretical calculations, we expect to gain deeper insights into phonon interactions influenced by moiré patterns. This research highlights the potential of twisted *h*-BN to probe new phenomena in two-dimensional materials and paves the way for further investigations into their complex properties.

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