Measuring the Surface Parameters of Metal Intercalated Graphene.

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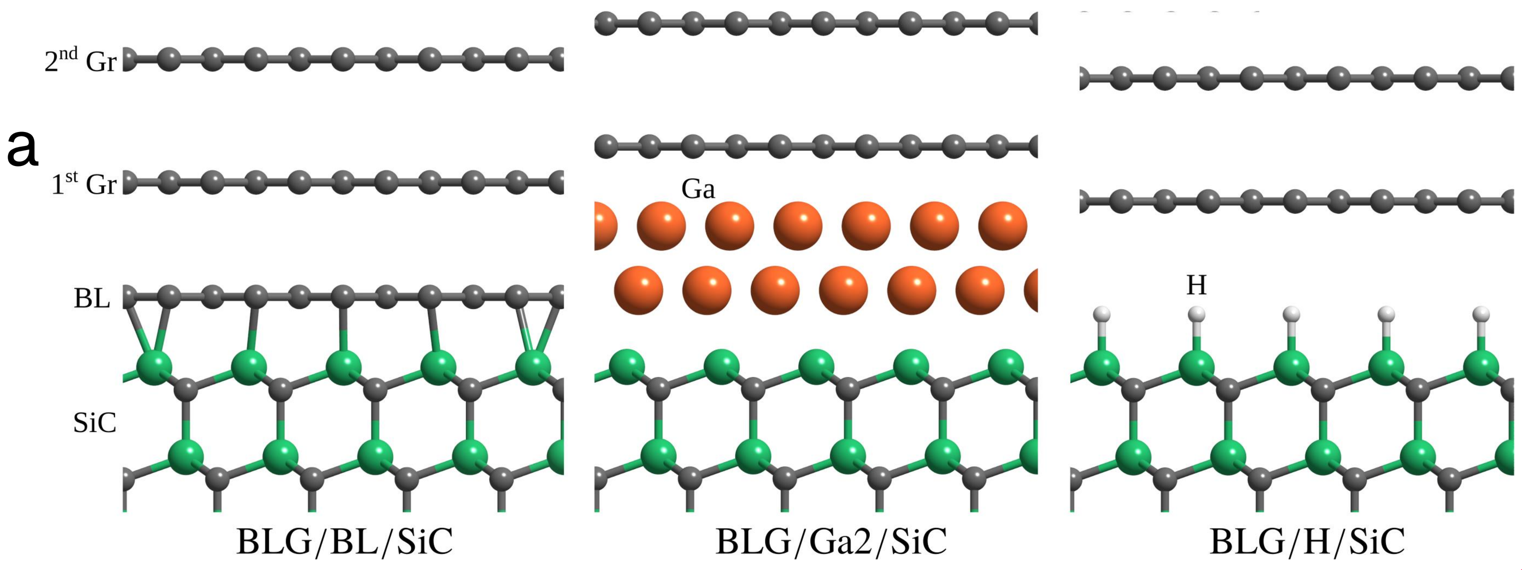


Introduction

- Helium atom scattering (HAS) is a purely surface sensitive, non-destructive technique that can be used to probe the properties of a material surface.
- Structural characteristics that can be investigated include the lattice constant, the linear thermal expansion coefficient (TEC), and the electronic corrugation.
- The technique can also be used to access intrinsic characteristics of the materials such as the electron-phonon (e-ph) coupling constant, λ_{HAS}.
- We investigate these properties for samples of epitaxially grown bilayer graphene (BLG) bound to various intermediate, intercalated substances atop a silicon carbide (SiC) substrate.

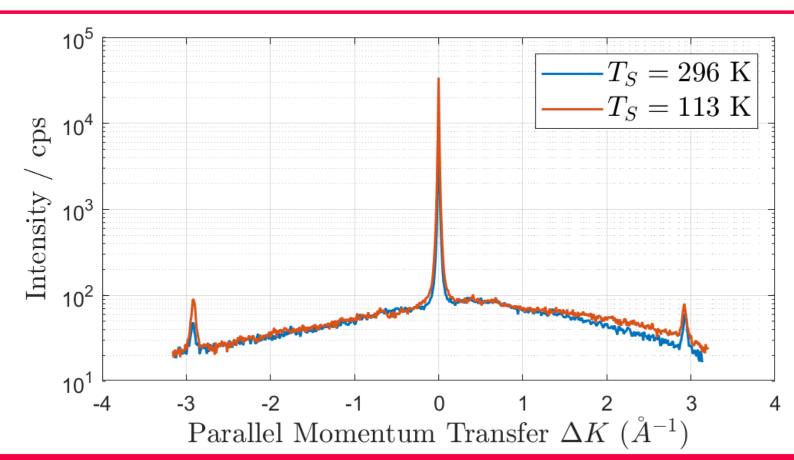
Surface Structure

- He beam diffraction patterns are generated according to the Laue condition.
- Using the angle of the first order diffraction peaks the reciprocal lattice constant of the graphene surface can be calculated.
- Taking the lattice constants at varying surface temperatures allows us to calculate the linear thermal expansion coefficient. These values are averaged across multiple He beam energies.

$$|G_{hk}| = 2|k_i|\cos\left(\frac{\vartheta_{SD}}{2}\right)\sin\left(\frac{\vartheta_{SD}}{2}-\vartheta_i\right) \quad ; \quad a = \frac{4\pi}{\sqrt{3}|G_{hk}|} \quad ; \quad \alpha_{\parallel} = \frac{\Delta a}{a_0 \Delta T_S}$$

- BLG exhibits a negative thermal expansion (NTE) which causes strain and potential slips or buckling when bound to substrates with positive thermal expansion such as SiC. [2]
- Slips and buckling are difficult to observe within our experiments due to the limited number of temperatures measured.

Sample	Lattice Constant (Å)		TEC ($\times 10^{-5}$ K $^{-1}$)
	113 K	296 K	
BLG/BL/SiC	2.480	2.468	-2.52
BLG/Ga_2/SiC	2.470	2.463	-1.37
BLG/H/SiC	2.486	2.472	-3.10



Electron Phonon Coupling

- As the surface of a material heats up more phonon modes become successively available.
- A greater proportion of the incident He beam undergoes inelastic scattering in place of elastic scattering.
- This is directly measurable via the thermal attenuation of the specular elastic peak intensity.

$$I(T_S) = I_0 \cdot e^{-2W(T_S)}$$

- Given that the He beam interacts exclusively with the electron density, and the exchange of energy occurs via phonon excitation there exists a coupling between the electrons and phonons described by the following equation,

$$2W(k_f, k_i, T_S) = 4\mathcal{N}(E_F)\left(\frac{mE_{iz}}{m_e^* \phi}\right)\lambda_{HAS} k_B T_S$$

- When applied to graphene at an arbitrary temperature, this becomes,

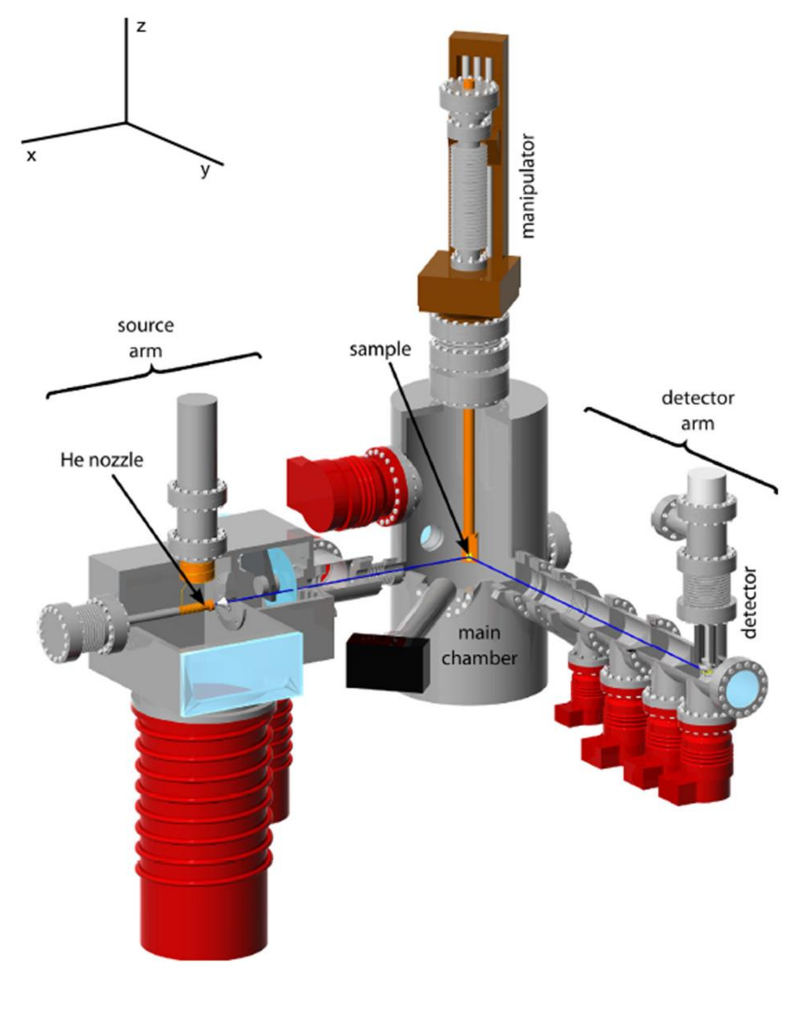
$$\lambda_{HAS}(T_S) = \frac{\pi\alpha}{2n_S} \quad ; \quad \alpha \equiv \frac{\phi \ln[I_0/I(T_S)]}{a_C k_{iz}^2 \hbar\omega_0 \left\{n_{BE}(\omega_0, T_S) + \frac{1}{2}\right\}} \qquad [4]$$

- λ_{HAS} has an inverse non-linear relationship with binding strength of the graphene to the substrate suggesting that intercalated Ga metal or, to a larger extent, H reduce the strength of the graphene binding.

Sample	BLG/BL/SiC	BLG/Ga_2/SiC	BLG/H/SiC	Gr/Ni(111) [5]	Gr/Ru(0001) [6]
$\lambda_{HAS}(\bar{T})$	0.089	0.091	0.100	0.06	0.05

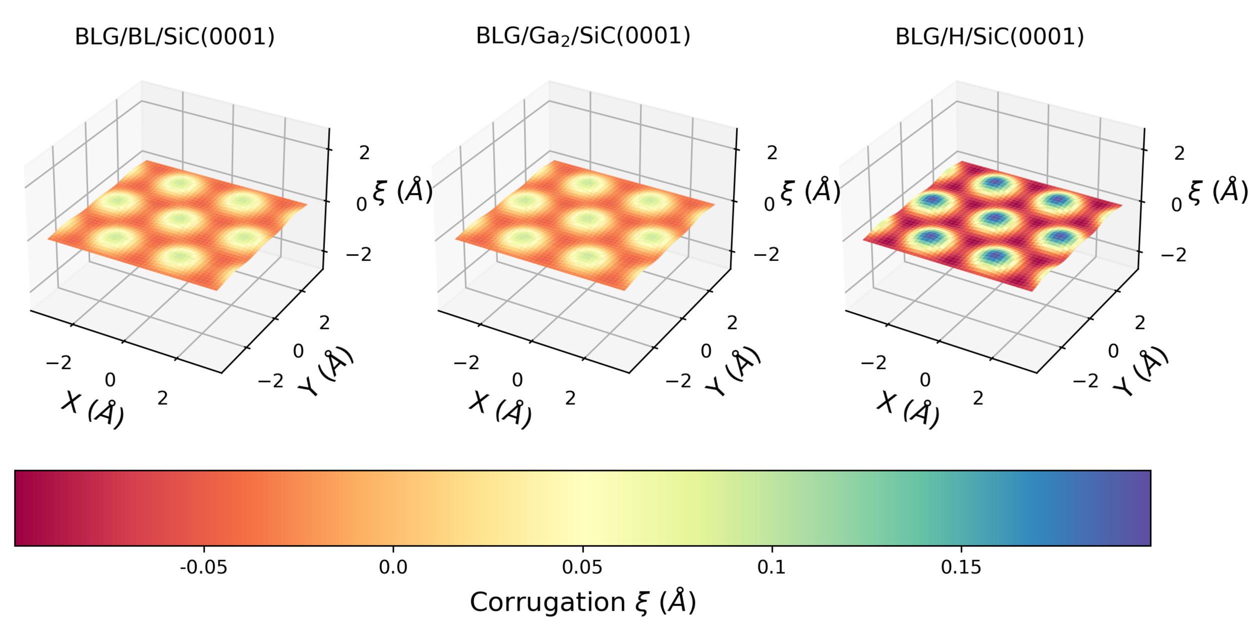
Experimental Setup

- Helium (He) atoms are accelerated via supersonic expansion through a temperature-controlled nozzle and collimating skimmer, generating a monochromatic ($^{\Delta E}/_{E} \approx 2\%$) He beam.
- The beam is directed towards a sample mounted to a manipulation arm.
- The low energy beam (8-13 meV) exclusively interacts with the electron cloud above the sample, without penetrating into the bulk.
- The diffracted beam is detected by a quadrupole mass spectrometer (QMS).
- There is a fixed angle between the He source and the detector, the angle of incidence can be adjusted by rotating the sample about the Z axis.
- $\vartheta_{SD} = \vartheta_i + \vartheta_f = 91.5°$
- The samples can be cooled to 113 K via a thermal connection to a liquid nitrogen reservoir.
- Further details are available in [1].



Electronic Corrugation

- The electronic corrugation is generated using purely elastic scattering, close-coupling (CC) calculations.
- The electronic corrugation of a surface influences the fraction of the incident He beam that is scattered into diffractive channels, and thus the intensity of the diffraction peaks.
- The peak-to-peak corrugations of the BLG/BL/SiC and BLG/Ga/SiC are relatively standard at 0.14 Å and in good agreement with BLG atop a Ru(001) surface at 0.15 Å. [3]
- The hydrogenated sample shows a more significant corrugation at 0.23 Å, surpassing even bulk highly-oriented pyrolytic graphite (HOPG) at 0.21 Å. [3]
- It is also notable that the corrugations become substantially stronger once the surfaces have been cooled, it is possible this is due to the reduced availability of phonon modes to facilitate inelastic scattering.



Acknowledgement & References

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