Quasi van der Waals epitaxy of GaAs on graphene/Si by molecular beam epitaxy

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III-V compounds epitaxially grown on silicon (Si) have attracted immense research interests for many years due to its applications in integration of optoelectronic devices with Si-based mature microelectronic technology. However, such direct heteroepitaxy is challenged by lattice mismatch, polar-on-nonpolar epitaxy, and thermal expansion mismatch. Quasi van der Waals epitaxial (QvdWE) growth of GaAs on Si using a two-dimensional layered material, graphene, as a lattice mismatch / thermal expansion coefficient mismatch relieving buffer layer is a novel route towards heteroepitaxial integration in the developing field of silicon photonics. In this study, we report the two-dimensional (2D) growth of GaAs thin films on graphene/Si system to create 3D/2D heterostructures. Here we show – for the first time - ultra-smooth morphology for GaAs films on silicon using QvdWE, making it a remarkable step towards an eventual demonstration of the epitaxial growth of GaAs by this approach.

Multilayer graphene (MLG) flakes were exfoliated on a bare Si wafer. The graphene flakes were then degassed in ultrahigh vacuum (UHV) at 300 °C for 10 min. The samples were left to be cooled down in vacuum prior to the growth. A Perkin-Elmer 430 molecular beam epitaxy (MBE) system was used to perform the growth. A cracked arsenic source was used in this system to produce As2. The growth was initiated by the deposition of gallium (Ga) prelayer at a temperature of 50 °C. Figure 1 shows a plan-view scanning electron microscope (SEM) image of GaAs grown on a Ga-terminated MLG surface at temperatures as low as 350 °C and a growth rate of 0.15 Å/s. For the first few layers, GaAs forms widely separated islands around nuclei, and the islands then coalesce as the growth proceeds. Figure 2 displays the atomic force microscope (AFM) image for GaAs films, showing surface RMS roughnesses as low as 0.6 nm, corresponding to around two monolayers of GaAs, as well as a peak-to-peak height variation of only 3 nm. This smooth low-temperature nucleation layer is considered to have an acceptable roughness for subsequent epitaxial growth of overlayers. Details will be discussed in the talk.

Ab-initio simulations of the GaAs/graphene/Si interface are performed to determine the interaction energy at the interface of this heterostructure. The impact of asymmetry in the grown GaAs layer (zinc-blende versus wurtzite) and rotational misalignment between GaAs and the graphene buffer layer on the interaction energy will be presented in the conference presentation.

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Fig. 1: SEM plan-view image of GaAs films grown with Ga-prelayer on multi-layer graphene/Si using V/III ratios of 25 and a growth rate of 0.15 Å/s, schematic cross-sectional view of the corresponding structure is shown as inset.

Fig. 2: AFM image of the 1.2 µm × 1.2 µm GaAs film grown with Ga-prelayer on multi-layer graphene/Si, showing the surface morphology.