

PCSI

Room Ballroom South - Session PCSI-SuE2

Novel Epitaxy

Moderator: Roman Engel-Herbert, Paul-Drude Institute for Solid State Electronics

8:10pm PCSI-SuE2-9 UPGRADED: Large Area Single Crystals of Borophene on Square- and Triangular-Lattice Metallic Surfaces: Synthesis and Characterization, *Adrian Gozar*, Fairfield University; *Ivan Beshpalov*, Caltech; *Jin Zhao*, Yale University; *Rongting Wu*, Chinese Academy of Sciences, China; *Ivan Bozovic*, Shanghai Advanced Research in Physical Sciences, China

The materials-by-design paradigm is based on synergistic efforts involving synthesis, characterization and advanced computation to ensure materials meet technological needs within a cost-effective framework. Borophene, a crystalline monolayer sheet, is envisaged to play an important role in this area because of its extraordinarily rich polymorphism. The multitude of potentially stable structures singles out borophene from all other two-dimensional materials and fuels hopes for obtaining on-demand structures with applications in flexible electronics, energy storage or catalysis.

We have used a unique ultra-high vacuum system for synthesis, by Molecular Beam Epitaxy, and in-situ characterization, by Low Energy Electron Microscopy, of micron-size borophene crystals on Cu(111) and Cu(100) substrates. Our real-time imaging capabilities provide information about the growth of faceted borophene islands up full monolayer coverage and also about phase-stability, evaporation and sub-surface dissolution. Combining low energy electron diffraction with scanning tunneling microscopy and ab initio theory allows us to resolve the crystal structures as triangular networks with vacancy ratios $\eta = 1/5$ for Cu(111) and $\eta = 1/6$ for Cu(100) surfaces. First-principles calculations indicate that charge transfer rather than covalent bonding, couples borophene to the underlying Cu surfaces. The calculated electronic band structures host multiple anisotropic Dirac cones. Ex-situ scanning near-field optical microscopy data reveal dielectric contrast between borophene and substrates, showing that nano-optical tools provide new ways to access intrinsic electronic properties of these novel structures.

8:30pm PCSI-SuE2-13 UPGRADED: Remote Epitaxial Frustration, *Jason Kawasaki*, University of Wisconsin Madison

Remote epitaxy promises to circumvent the lattice and chemical mismatch challenges of conventional epitaxy, to enable low defect density and chemically abrupt heterostructures of dissimilar materials. However, definitive experimental evidence for a true "remote" mechanism remains elusive because most observations can be explained by alternative pinhole or van der Waals mechanisms, which are often macroscopically indistinguishable from a true "remote" mechanism. Here, using GdAuGe films grown on graphene/SiC (0001), we present two long-range signatures of a remote mechanism that cannot be explained by the leading alternatives: (1) a two atomic layer thick disordered interlayer at the GdAuGe/graphene interface and (2) a new 30° rotated epitaxial relationship between GdAuGe film and SiC substrate. Density functional theory calculations suggest that these signatures arise from remote epitaxial "frustration," i.e. a competition between epitaxy of the GdAuGe film to the screened remote potential of the substrate (φ_{sub}), versus direct epitaxy to graphene (φ_{gr}) and to the long-range graphene-induced surface reconstruction (φ_{rec}). Our results highlight the importance of considering the multiple contributions to the total lattice potential above graphene-covered surfaces, rather than an exclusive focus on φ_{sub} . Moreover, tuning the relative magnitude and periodicities of φ_{gr} , φ_{sub} , and φ_{rec} provides new opportunities to (1) control short- and medium-range ordering of films stabilized at graphene-covered interfaces, towards the discovery of new glasses and quasicrystals, and (2) direct synthesis of rotated moire heterostructures for tuning magnetism and correlated phases

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