van-der-Waal materials as buffer layers for quasi-vdW epitaxy of GaAs on Si

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Epitaxial growth of III-V compounds on silicon (Si) would enable the integration of CMOS devices and optoelectronic devices. However, direct heteroepitaxy faces challenges of lattice mismatch, polar-on-nonpolar epitaxy, and thermal expansion mismatch. A buffer layer of multi-layer graphene was recently used to alleviate the mismatch in lattice constants and thermal expansion coefficients by achieving quasi van der Waals epitaxial (QvdWE) growth of thin-film GaAs on Si[i]. Ab-initio electronic structure calculations are used to determine the interaction energy at the GaAs/graphene heterointerface. Crystal asymmetry between graphene and the grown GaAs layer (zinc-blende versus wurtzite) and rotational misalignment between GaAs and the graphene buffer layer alter the interaction energy. The GaAs(111) zinc-blende (ZB) phase is the preferred orientation of growth on graphene. The binding energy of ZB GaAs(111) on graphene is maximum for misorientation angles $13^0 < \theta < 30^0$ and is minimum for the perfectly aligned interface. The binding energy of ZB GaAs(111) on alternative van-der-Waals materials (h-BN, MoS_2, GaSe) is lower than the binding energy of ZB GaAs(111) on graphene.

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[i] Yazeed Alaskar, Shamsul Arafin, Darshana Wickramaratne, Mark A. Zurbuchen, Liang He, Jeff McKay, Qiyin Lin, Mark S. Goorsky, Roger K. Lake, and Kang L. Wang. "Towards van der Waals Epitaxial Growth of GaAs on Si using a Graphene Buffer Layer." *Advanced Functional Materials* 24, no. 42 (2014): 6629-6638.