Two-dimensional optoelectronic integration with silicon systems

Mike Cooke reports on proposals and explorations of the potential of combining graphene, transition metal dichalcogenides, and hexagonal boron nitride with complementary metal-oxide-semiconductor electronics.

As global communication networks and remote storage facilities expand, the demand is for broader bandwidths and high-speed computer processing with low power consumption. Optical communications offer high data rates with low transmission decay. As purely electronic systems reach physical atomic limits, such systems are being combined with optical communications — both long-haul, and increasingly board-to-board, or even chip-to-chip. As always, these developments must be aimed at power-efficient performance at low cost.

Researchers are seeking photonic integrated circuits on silicon platforms using processes compatible with complementary metal–oxide–semiconductor (CMOS) technology. An important class of materials consists of few-layer or even one-layer two-dimensional (2D) lattices of elements. The archetypal example is graphene (G), consisting of carbon atoms in a hexagonal formation with so-called sp^2 bonding. More recently, transition-metal dichalcogenides (TMDs, MX_2) have come to prominence in the research literature.

Bulk TMDs tend to have indirect bandgaps, but mono-/few-layer versions often have the direct transitions needed for efficient light emission and detection. The metal 'M' parts of the MX_2 chemical formula can be molybdenum (Mo), tungsten (W), tantalum (Ta), titanium (Ti) or niobium (Nb). The dichalcogenic 'X_2' part is supplied by sulfur (S), selenium (Se) or tellurium (Te). There are also possibilities of compounding group III elements gallium and indium with chalcogenic elements (GaX, In_2X_3).

Tianhua Ren and Kian Ping Loh of National University of Singapore [J. Appl. Phys., vol125, p230901, 2019] comment: "Two-dimensional transition-metal dichalcogenides are attractive candidates as on-chip emitters and absorbers due to their direct bandgaps, compatibility with miniaturization, large exciton binding energies, anisotropic polarizations, and strong light-matter interactions."

Unfortunately, direct growth of TMDs and related materials on silicon or silicon dioxide (SiO_2) is still a bottleneck. Most research uses laborious techniques such as mechanical exfoliation of TMD flakes with sticky 'Scotch Tape' and manual manipulation, which are not suitable for precision mass production.

The different 2D (i.e. mono- or few-layer) TMDs can provide various metal, semi-metal and semiconductor electrical transport. Ren and Loh favor hexagonal boron nitride (hBN) as an insulator material and for waveguide cladding/optical confinement. "On-chip integrated photonic circuits are proposed based on heterostructures of hexagonal boron nitride and two-dimensional materials with functions of light sources, optical modulators, and photodetectors toward high-bandwidth optical interconnects," they report.

hBN has been reported with an in-plane refractive index of 2.3, compared with silicon dioxide's less than 1.5 at visible and near-infrared wavelengths. This contrast is one way to provide light confinement. Further confinement could be achieved in hBN/TMD/hBN stacks, with Van der Waals (VdW) bonding between the layers, creating opportunities to create optical cavities for laser and other emission and detection schemes. Although some work has already used such structures, problems arose from 0.7–4.8eV mid-gap energy levels, arising from crystal defects in the hBN.

Ren and Loh envisage vertical confinement arising from the refractive index contrast between hBN and silicon dioxide substrates/templates and top layers. Horizontal confinement could be achieved with patterning and etching mesa or photonic crystal/air-hole 2D lattice structures.

Light-emitting diodes

Proposals for TMD LEDs come in two forms: lateral and vertical. In the lateral setup, the p- and n-doped regions of the LED are placed side-by-side, creating carrier sources for recombination in the region/junction between the doped materials. The vertical structure instead places the doped material in a stack — a form familiar from the epitaxial growth of III-V LEDs.

Some 2D TMD LEDs have already been reported, such as the first such device in 2013. This LED consisted of a Schottky junction between MoS_2 and chromium/gold. Attempts to use electrostatic doping to give p- and n-type regions failed on this occasion. The external quantum efficiency (EQE) of the Schottky junction was a very low 10^{-5}. Higher EQEs of up to 10% were achieved with vertical stacks using naturally n-type MoS_2 and p-WSe_2 in 2014.

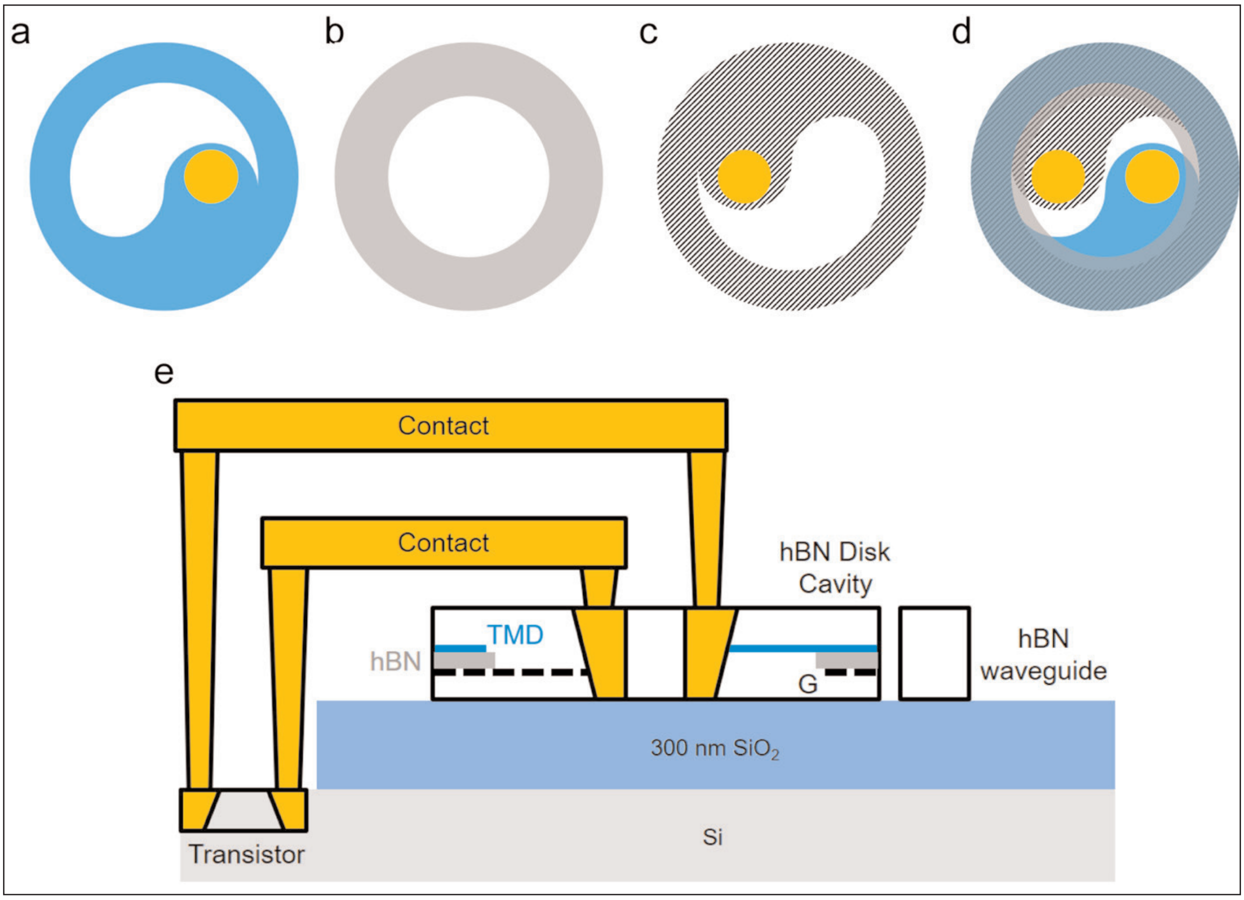

Figure 1. Schematic design of proposed LED with hBN disk cavity. Top view patterns of (a) top TMD layer, (b) middle hBN layer, (c) bottom graphene (G) layer, and (d) TMD/hBN/graphene trilayer; (e) side view of LED structure connected with silicon transistor.

Ren and Loh suggest that a cavity-enhanced LED could be constructed using a graphene/hBN/TMD stack as the active region (Figure 1). By applying differently shaped layers extending from a ring of material, an hBN cavity with whispering gallery modes that couple with the active junction is formed. The researchers suggest that, with a high enough quality-factor cavity, laser action could be possible. Metal interconnects could link the diode electrodes to silicon CMOS circuitry.

Optical modulators and detectors

Moving on to the original 2D material (graphene), Ren and Loh see — among its other potentials — the use of its refractive-index modulation by electrostatic doping via top or bottom gate structures in optical modulator stages, giving amplitude and phase manipulation. Mach–Zender interferometers have been realized with 35dB modulation and 5GHz bandwidth using a gate swing of the order of 2V, rather than the typical 10–50V in amplitude modulators. Ren and Loh comment: “The real-world application of 100GHz bandwidth optical interconnects should require multiplexing of wavelengths using multi-channels of graphene optical modulators.”

Again, Ren and Loh want to combine graphene modulation with an hBN cavity structure. The modulation would be achieved by an aluminium oxide layer sandwiched between graphene layers, and strongly coupled to the whispering gallery modes of the hBN cavity.

TMDs have also been used as the basis of the easier photodetector function using either metal–semiconductor–metal (MSM) or photovoltaic structures.

MSM devices have demonstrated high response (the current for a given light power), but the bandwidth for detecting modulated signals is limited. Increasing the bandwidth requires boosting mobility and improving crystal quality. By contrast, graphene-based MSM devices tend to have high bandwidth but poor response. Also, multi-layer TMD detectors have improved bandwidth at the cost of reduced response. MSM detectors have been realized in both lateral and vertical formats.

Photovoltaic detectors based on pn-junction separation of the generated carriers offer reduced dark current in reverse-bias mode. Again, Ren and Loh propose using hBN cavities to enhance the detector performance. At present, they favor a graphene/TMD/graphene sandwich as the detector component due to its potential for GHz-level bandwidths.

Ren and Loh see their hBN cavity components as forming an electronic-photonic-electronic chain:

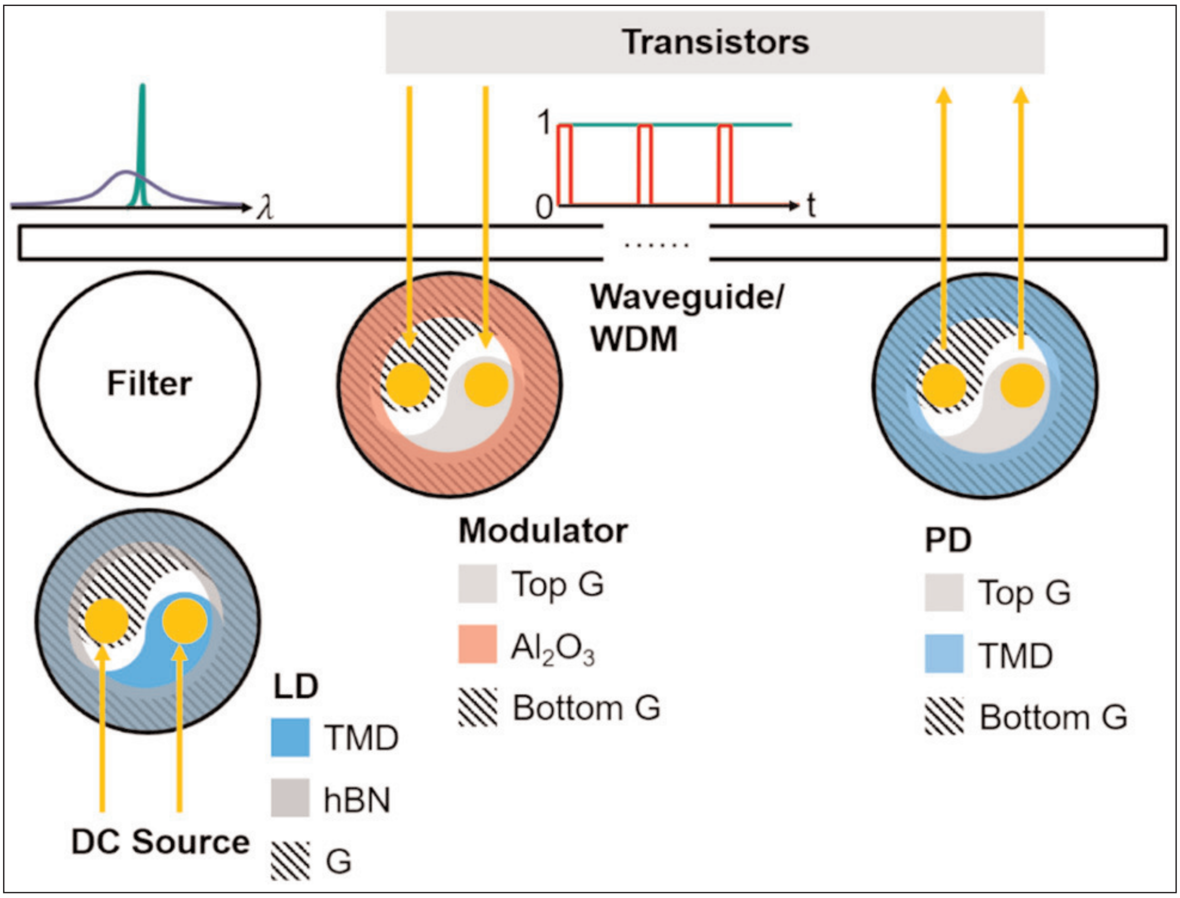

Figure 2. Integrated photonic circuits with hBN disk cavity and waveguide on SiO_2/Si platform.

Ren and Loh admit: "The practical realization of these photonic circuits requires the monolithic growth of large-area TMD and hBN on the silicon platform, which has yet to be achieved to date. Nonetheless, breakthroughs in large-area TMD and hBN growth have been achieved on other substrates; thus, future developments in automated wafer-to-wafer transfer techniques may help address the gap in materials integration."

graphene/hBN/TMD laser diode/LED, filtering to a single wavelength with a passive hBN cavity with continuous output, modulation into wavelength division multiplex (WDM) signals, transmission by waveguide/optical fiber, and detection with photodetectors (Figure 2).

Visualization

TMDs, graphene and hBN also feature in the work of a group of researchers based in the USA, the UK and Italy who have used 2D VdW graphene/hBN/graphite heterostructures to realize micron-scale, angle-resolved photoemission spectroscopy (microARPES) as a platform for investigating the electronic structure of graphene and TMDs [Paul V Nguyen et al, Nature, online 17 July 2019].

The team from University of Washington (USA), University of Warwick (UK), Elettra-Sincrotrone Trieste SCpA (Italy) and University of Cambridge (UK) comments: "The technique provides a powerful way to study not only fundamental semiconductor physics, but also intriguing phenomena such as topological transitions and many-body spectral reconstructions under electrical control."

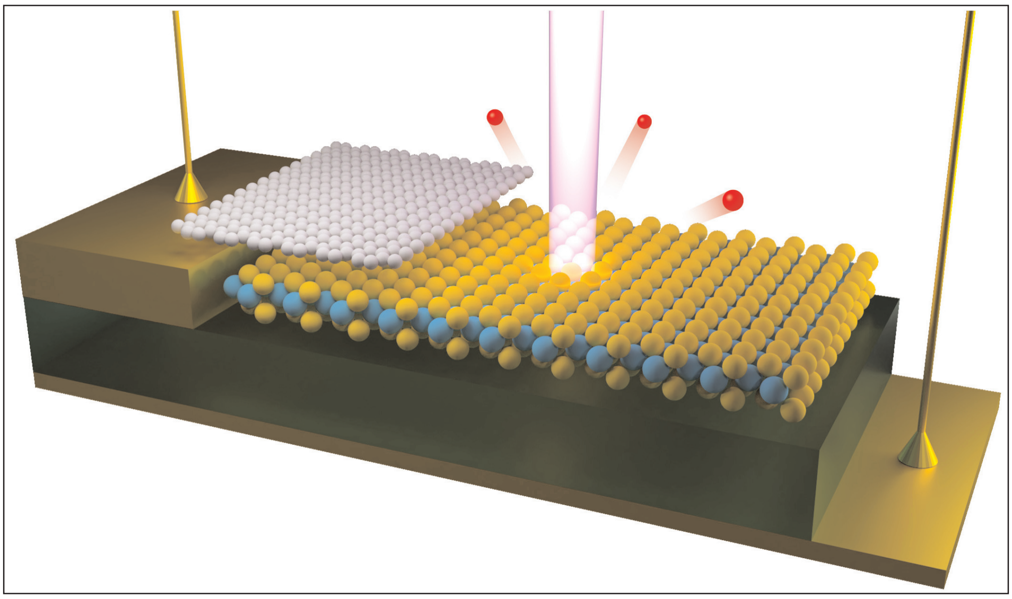

Figure 3. Electrons ejected by a beam of light focused on two-dimensional semiconductor device are collected and analyzed to determine how electronic structure in material changes as voltage is applied between electrodes. Credit: Nelson Yeung/Nick Hine/Paul Nguyen/David Cobden.

ARPES techniques use narrow-spectrum ultraviolet or x-radiation to eject electrons from samples (Figure 3). The direction and energy of these electrons provide information about energy levels within the sample of interest. ARPES tends to only give data on near surface levels, so it is generally not that useful for bulk properties. However, 2D materials such as graphene and TMDs are essentially all about surface states.

Recently, focusing techniques such as Schwarzschild objectives, Fresnel zone plates, and capillary mirror optics have enabled focusing of synchrotron beam-lines to provide the micron-scale spots needed for microARPES. The researchers used a Schwarzschild objective to focus radiation produced at the Elettra synchrotron facility in Italy. The photon energy was mainly 27eV.

Since ARPES sees only filled levels, doping techniques are needed to explore the conduction band. The researchers used electrostatic doping with a gate potential applied to the graphite underlayer, rather than introducing chemical impurities.

The researchers were particularly keen to explore the directness of the conduction band edge (CBE) in monolayer and few-layer 2D materials. It is thought that monolayers of many TMDs such as WSe_2 have a direct gap at the corner of the hexagonal Brillouin zone, designated as 'point K', rather than at the central 'Γ point' (Figure 4). The directness arises since the valence band is highest at point K. As one adds layers an intermediate valley at the less symmetric 'point Q' between K and Γ reduces in energy and the gap becomes indirect.

The team reports: "Using electrostatic doping in microARPES, we confirm that the CBE is at K in all of the monolayer semiconductors — MoS_2, $MoSe_2$, WS_2 and WSe_2 — and in each case we obtain a measure of the bandgap. We also study the layer-number dependence in WSe_2, finding that the CBE moves to Q in the bilayer, and measure for the first time the renormalization of the band structure on gating." ■

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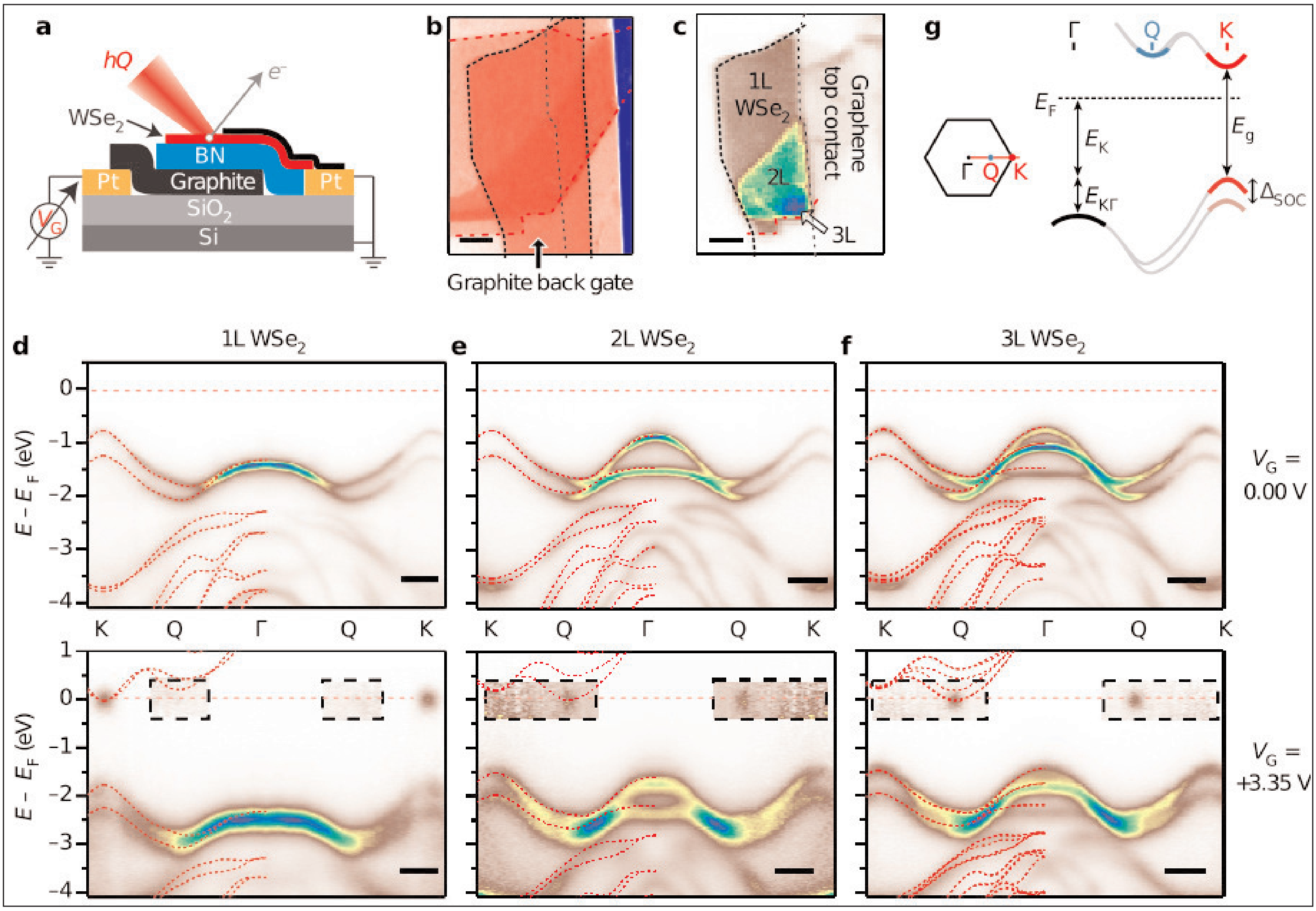

Figure 4. (a) Diagram of device incorporating WSe_2 flake, with overlapping ground graphene top contact and gate voltage applied to graphite back gate. Optical (b) and scanning photoemission microscopy (c) images of WSe_2 device (hBN thickness 7.4nm), with monolayer (1L), bilayer (2L) and trilayer (3L) regions identified. Scale bars, 5μm. (d–f) Energy-momentum slices along Γ–K for 1L, 2L and 3L regions, respectively. Upper panels are at 0V gate and lower ones at +3.35V. Intensity in dashed boxes multiplied by 20. Fuzzy spots signal population of CBE. Scale bars, 0.3/Å. Data reflected about Γ to aid comparison with electronic structure calculations (GW self-energy approximation to first term of Green function (G) and screened Coulomb interaction (W); red dashed lines). (g) Brillouin zone of MX_2 (left) and diagram of bands along Γ–K (right), showing definitions of energy parameters.