TWO-DIMENSIONAL MATERIALS

Leaving defects out of 2D molybdenum disulfide

By incorporating oxygen into the chemical vapour deposition growth of molybdenum disulfide, sulfur vacancies can be passivated and contact resistances lowered.

Saptarshi Das and Ana Laura Elías

Two-dimensional (2D) materials can behave as insulators, conductors and semiconductors, and are of potential use in a growing range of applications, from electronics to catalysis to energy storage. In the development of such applications, the identification and understanding of defects is an important issue[1]. Point defects, such as chalcogen vacancies in semiconducting transition metal dichalcogenides, have, for instance, been identified as one of the causes of low performance in electronic devices based on 2D materials[2]. But, at the same time, defects can also be used to manipulate the physical properties of the materials and create tailored applications. The defect-mediated functionalization of 2D materials has, for example, been used to obtain dilute magnetic semiconductors with ferromagnetic order at room temperature for applications in magnetoelectric devices[3]. Alternatively, defect migration between electrodes[4] and defect-induced trapping and detrapping of charge carriers[5] have been used to develop novel forms of computing — including neuromorphic, bioinspired and biomimetic[6] — with 2D materials.

Defect engineering via chemical doping can be used to tune the properties of 2D semiconductors[1]. This can be done after the growth of the 2D materials, or during the growth process itself. An advantage of doping during growth is that the dopant atoms can be covalently bonded to the crystalline lattice, making the doping more resilient to subsequent fabrication processes (which can involve harsh wet chemistries and environments)[3]. Covalently bonded oxygen can, in particular, be used to passivate native chalcogen monovacancies — sulfur vacancies in the case of molybdenum disulfide (MoS_2) — which are common defects in the crystalline lattice of some 2D materials. Writing in *Nature Electronics*, Jing Kong and colleagues now report an approach for passivating sulfur vacancies in MoS_2 using an oxygen-incorporated chemical vapour deposition process to grow the materials[7]. Field-effect transistors (FETs) built with the resulting 2D materials offer enhanced capabilities compared with devices built with materials grown via standard methods.

Two-dimensional semiconductors have been proposed as an alternative for silicon as the channel material of scaled FETs[8]. But for this to be possible, it will be essential to eliminate native defects in the 2D materials or minimize their impact on electronic transport (Fig. 1). For example, a high density of chalcogen vacancies and other structural defects impedes the formation of ohmic contacts at the metal/semiconductor interfaces and leads to a high contact resistance[9]. Chalcogen vacancies also act as scattering sources, leading to reduced carrier mobility and unintentional doping, which result in large device-to-device variation[2], or as trapping centres, leading to hysteresis and a poor subthreshold slope. Furthermore, the study of deep states in semiconducting transition metal dichalcogenides, such as the recently reported room-temperature DX centre defects in molybdenum disulfide and tungsten disulfide[10], is needed to bring 2D semiconducting materials closer to application.

Kong and colleagues — who are based at the Massachusetts Institute of Technology, Mount Holyoke College, Boston University and Tsinghua University — used an oxygen-incorporated chemical vapour deposition technique that passivates sulfur vacancies and suppresses the formation of donor states in MoS_2. Experimental and computational work by the researchers on the configuration of the defects shows that this was due to the formation of molybdenum–oxygen bonding at the vacancy site. This reduces the Schottky barrier and lowers the metal/MoS_2 contact resistance to around 1 kΩ μm. Additionally, gate-dependent photoluminescence measurements on the passivated MoS_2 show no emission originating from defect-bound excitons.

While lowering contact resistance is an important step in the development of 2D electronics, further work is needed to meet the strict requirements of the International Roadmap for Devices and Systems (IRDS)[8], which are necessary for the integration of 2D

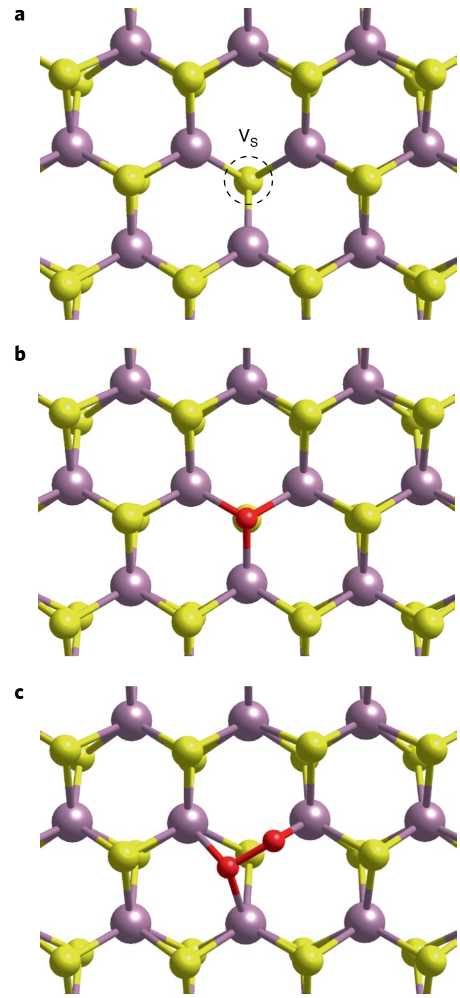

Fig. 1 | Schematic of the atomic structure of molybdenum disulfide. a, Atomic structure of MoS_2 containing a sulfur vacancy (V_s), resulting in donor-like states in the band structure. **b**,**c**, The addition of a single oxygen atom (**b**) and two oxygen atoms (**c**) to the V_s site, via oxygen-incorporated chemical vapour deposition, removes the induced defect states and introduces additional acceptor-like states. Purple, molybdenum atoms; yellow, sulfur atoms; red, oxygen atoms. Figure adapted with permission from ref. [7], Springer Nature Ltd.

materials in large-scale integrated circuits. This will require a more precise control of all fabrication steps and a deeper understanding of defects in 2D semiconducting materials. And the challenge demands the further development of growth methods and large-scale structural characterization, which should be done in combination with spectroscopic and electronic transport measurement techniques. ❐

Saptarshi Das [1] ✉ and
Ana Laura Elías [2] ✉

[1]*Department of Engineering Science and Mechanics, Department of Materials Science and Engineering, Materials Research Institute, Pennsylvania State University, University Park, PA, USA.* [2]*Department of Physics, Binghamton University, Binghamton, NY, USA.*
✉*e-mail: sud70@psu.edu; alelias@binghamton.edu*

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References

1. Lin, Z. et al. *2D Mater.* **3**, 022002 (2016).
2. Sebastian, A., Pendurthi, R., Choudhury, T. H., Redwing, J. M. & Das, S. *Nat. Commun.* **12**, 693 (2021).
3. Zhang, F. et al. *Adv. Sci.* **7**, 2001174 (2020).
4. Sangwan, V. K. et al. *Nature* **554**, 500–504 (2018).
5. Arnold, A. J., Razavieh, A., Nasr, J. R., Schulman, D. S., Eichfeld, C. M. & Das, S. *ACS Nano* **11**, 3110–3118 (2017).
6. Cao, G. et al. *Adv. Funct. Mater.* **31**, 2005443 (2021).
7. Shen, P.-C. et al. *Nat. Electron.* https://doi.org/10.1038/s41928-021-00685-8 (2021).
8. IEEE International Roadmap for Devices and Systems (IRDS, 2020); https://irds.ieee.org/editions/2020
9. Schulman, D. S., Arnold, A. J. & Das, S. *Chem. Soc. Rev.* **47**, 3037–3058 (2018).
10. Ci, P. et al. *Nat. Commun.* **11**, 5373 (2020).

Competing interests

The authors declare no competing interests.