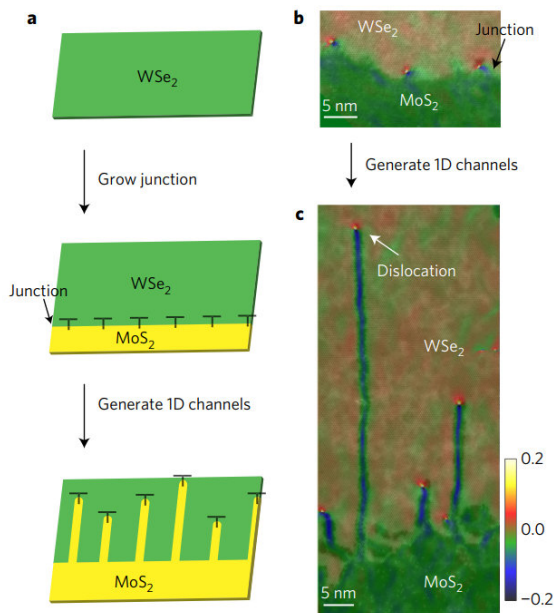


Subnanometer-scale channels in 2-D materials could point toward future electronics, solar cells

4 December 2017



Formation of 1D channels. a, Schematic of the patterning process guided by misfit dislocations (marked as 'T') at the MoS₂–WSe₂ lateral heterojunction. b,c, Atomic-resolution ADF-STEM images overlaid with their ϵ_{xx} strain maps (see Fig. 2 for more details) identifying the periodic dislocations at the interface of MoS₂ and WSe₂ (b) and the 1D channels created by chemically driven migration of the interfacial dislocations as additional S and Mo atoms are added (c). Strain maps refer to the WSe₂ lattice. Credit: *Nature Materials* (2017). doi:10.1038/nmat5038

"Two-dimensional materials"—materials deposited in layers that are only a few atoms thick—are promising for both high-performance electronics and flexible, transparent electronics that could be layered onto physical surfaces to make computing ubiquitous.

The best-known 2-D material is graphene, which is a form of carbon, but recently researchers have

been investigating other 2-D [materials](#), such as [molybdenum disulfide](#), which have their own, distinct advantages.

Producing useful electronics, however, requires integrating multiple 2-D materials in the same plane, which is a tough challenge. In 2015, researchers at King Abdullah University in Saudi Arabia developed a technique for depositing molybdenum disulfide (MoS₂) next to tungsten diselenide (WSe₂), with a very clean junction between the two materials. With a variation of the technique, researchers at Cornell University then found that they could induce long, straight wires of MoS₂—only a few atoms in diameter—to extend into the WSe₂, while preserving the clean junction.

The researchers contacted Markus Buehler, the McAfee Professor of Engineering in MIT's Department of Civil and Environmental Engineering, who specializes in atomic-level models of crack propagation, to see if his group could help explain this strange phenomenon.

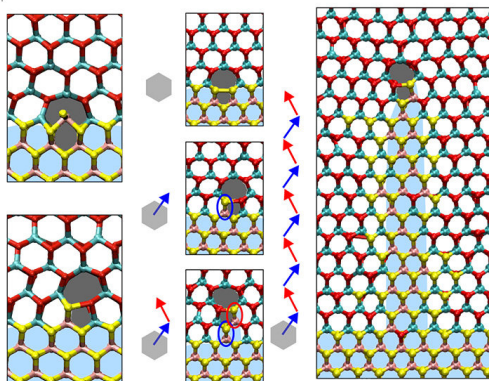
In the latest issue of *Nature Materials*, the King Abdullah, Cornell, and MIT researchers team with colleagues at Academia Sinica, the Taiwanese national research academy, and Texas Tech University to describe both the material deposition method and the mechanism underlying the formation of the MoS₂ nanowires, which the MIT researchers were able to model computationally.

"The manufacturing of new 2-D materials still remains a challenge," Buehler says. "The discovery of mechanisms by which certain desired material structures can be created is key to moving these materials toward applications. In this process, the joint work of simulation and experiment is critical to make progress, especially using molecular-level models of materials that enable new design

directions."

Wired up

The ability to create long, thin MoS₂ channels in WSe₂ could have a number of applications, the researchers say.



A slight mismatch between the hexagonal structures of molybdenum disulfide and tungsten diselenide creates a strain that can be released by the formation of a "5|7 dislocation," in which two hexagons collapse to form a pentagon and a heptagon. Reactions with molybdenum disulfide in the environment cause the dislocation to move deeper into the tungsten diselenide, drawing a nanowire of molybdenum disulfide behind it. Credit: Massachusetts Institute of Technology

"Based on [the materials'] electrical properties and optical properties, people are looking at using MoS₂ and WSe₂ for solar cells or for water splitting based on sunlight," says Gang Seob Jung, an MIT graduate student in civil and [environmental engineering](#) and a coauthor on the new paper. "Most of the interesting stuff happens at the interface. When you have not just the one interface—if there are many nanowire interfaces—it could improve the efficiency of a solar cell, even if it's quite random."

But the theoretical explanation of the molecular mechanism underlying the nanowires' formation also raises the hope that their formation could be controlled, to enable the assembly of atom-scale

electronic components.

"Two-D materials, one of the most promising candidates for future electronics, ultimately need to beat silicon-based devices, which have achieved a few nanometers in size already," says Yimo Han, a Cornell [graduate student](#) in chemistry and first author on the paper. "Two-D materials are the thinnest in the vertical direction but still span a quite large area in the lateral dimensions. We made the thinnest dislocation-free channels in 2-D materials, which is a big step toward subnanometer electronic devices out of 2-D materials."

Propagating polygons

In a 2-D crystal, both MoS₂ and WSe₂ naturally arrange themselves into hexagons in which the constituent elements—molybdenum and sulfur or tungsten and selenium—alternate. Together, these hexagons produce a honeycomb pattern.

The Cornell researchers' fabrication technique preserves this honeycomb pattern across the junction between materials, a rare feat and one that's very useful for electronics applications. Their technique uses chemical vapor deposition, in which a substrate—in this case, sapphire—is exposed to gases carrying chemicals that react to produce the desired materials.

The natural sizes of the MoS₂ and WSe₂ hexagons are slightly different, however, so their integration puts a strain on both crystals, particularly near their junction. If a pair of WSe₂ hexagons right at the MoS₂ junction convert into a hexagon matched with a heptagon (a seven-sided polygon), it releases the strain.

This so-called 5|7 dislocation creates a site at which an MoS₂ particle can attach itself. The resulting reaction inserts a molybdenum atom into the pentagon, producing a hexagon, and breaks the heptagon open. Sulfur atoms then attach to the heptagon to form another 5|7 dislocation. As this process repeats, the 5|7 dislocation moves deeper into WSe₂ territory, with a nanowire extending behind it. The pattern in which the strain on the mismatched hexagons relaxes and recurs ensures that the dislocation progresses along a straight line.

More information: Sub-nanometre channels embedded in two-dimensional materials, *Nature Materials* (2017).

[nature.com/articles/doi:10.1038/nmat5038](https://doi.org/10.1038/nmat5038)

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