2-D materials' crystalline defects key to new properties

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Understanding how atoms "glide" and "climb" on the surface of 2D crystals like tungsten disulphide may pave the way for researchers to develop materials with unusual or unique characteristics, according to an international team of researchers.

"If we don't understand what is behind the materials' characteristics caused by these defects, then we can't engineer the right properties into devices," said Nasim Alem, assistant professor of materials science and engineering, Penn State. "With a closer look, we might find that some of the defects are no good, that we don't want them in our materials, but we need to understand the defects first."

Tungsten disulphide as a 2D crystalline material is a semiconductor, so it can be used in electronic devices and it is also a catalyst used to liberate hydrogen gas from compounds. The defects or dislocations occur when an atom is displaced from the regular, repeated pattern of atoms in the crystal.

A key to understanding how the defects influence material behavior is to be able to see them. The researchers looked at tungsten disulphide, which is a three atomic layer, two-dimensional material, using an aberration-corrected scanning transmission electron microscope at the National Center for Electron Microscopy, Lawrence Berkeley National Laboratory.

"We can image atoms in the crystal and the way they move with the electron microscope," said Alem.

The researchers note in a recent issue of *Nature Communications* that "direct atomic-scale imaging coupled with atomistic simulations reveals a strikingly low-energy barrier for glide, leading to significant grain boundary reconstruction in tungsten disulphide."

In other words, defects in this material can easily be displaced to another location. This is different from similar investigations done on graphene, a more familiar 2D material made of carbon atoms. Since these defects are on the surface of the crystal, when they form they can change the shape of the crystal. "This can allow us to use of defects and dislocations to create new shapes in these crystals," said Alem.

"This microscopic approach is very interesting," said Alem, who notes that Penn State will soon have a working aberration-corrected scanning transmission electron microscope in its Millennium Science Complex. "It's like putting on a set of goggles and seeing things we haven't been able to see before. It's bringing new physics and mechanics to bear that people thought about, but we are now able to directly examine."

The researchers also looked at the strain that dislocations cause in the materials, determining that these defects can produce significant amounts of strain that need to be considered in materials preparation and use.

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