Strong elasticity size effects in ZnO nanowires

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Recently, zinc oxide (ZnO) nanowires have drawn major interest because of their semiconducting nature and unique optical and piezoelectric properties. Various applications for ZnO nanowires have been conceived, including the next generation of field effect transistors, light emitting diodes, sensors and resonators. ZnO nanowires are also envisioned as nanogenerators by exploiting the coupling of semiconducting and piezoelectric properties.

Researchers at the McCormick School of Engineering and Applied Science at Northwestern University recently performed experiments and computations to resolve major existing discrepancies about the scaling of ZnO nanowires elastic properties. These properties are essential to the design of reliable novel ZnO devices, and the insight emerging from such studies advances scientific understanding about atomic structures, which are also responsible for piezo-electric and piezo-resistive properties.

ZnO nanowires usually have a hexagonal cross-section, with diameters ranging from 5 to 500 nanometers. Interesting changes in their properties arise as the diameter of the wires decreases due to increasing surface-to-volume ratio. Unfortunately, experimental results reported in the literature on wire elasticity for a given diameter exhibit a large variability.

"This highlights one of the major challenges in the field of nanotechnology — the accurate measurement of nanoscale mechanical properties," says Horacio Espinosa, professor of mechanical engineering at McCormick. "Indirect measurement techniques and ill-defined boundary conditions affected mechanical properties measurements and resulted in problematic inconsistencies."

Espinosa and his group at Northwestern resolved this discrepancy using a nanoscale material testing system based on microelectromechanical system (MEMS) technology. The system was used to perform in-situ electron microscopy tensile testing of nanowire specimens. Load and displacements were measured electronically while the deforming material was imaged with atomic resolution.

"Direct atomic imaging was instrumental in assessing the effectiveness of the test," Espinosa says.

The experimental findings revealed that the elastic stiffness of ZnO nanowires monotonically increases as their diameter decreases. Atomic level computational studies were also conducted to identify the reasons for the observed size effect.

"Our experimental method is the most direct and simplest in terms of data interpretation," says Bei Peng, a McCormick graduate student and co-author of the paper. "We feel quite certain on all the quantities we have measured. Moreover, the fact that the experimental trends and atomistic predictions agree is quite rewarding."

In this research article, the reason for the observed size dependence was also reported.

"Atoms on the surface of the wires are rearranged because they have fewer neighboring atoms as compared to atoms in the core of the nanowire," says Ravi Agrawal, a McCormick graduate student and co-author of the paper. "The resulting surface reconstruction leads to wire material properties very different to that encountered in bulk."

This phenomenon has been observed previously for various metallic nanowires with large surface-to-volume ratios, but the surface effect was confined to wires with diameters smaller than approximately 10 nm.

"Due to the ionic character of ZnO, the atoms interact via electrostatic forces, which are long-range in nature. Therefore, the size effect is found to be significant up to nanowires with diameters of about 80 nm," says Eleftherios Gdoutos, an undergraduate student and co-author of the paper.

"Our research approach based on a combined experimental-computational investigation of the mechanics of nanowires is very promising," Espinosa says. "We are currently employing MEMS devices that allow piezo-electric and piezo-resistive characterization of semiconducting nanowires. We are also investigating the effect of the identified atomic surface reconstruction on polarization and energy bands, which should impact piezo-electricity and electric conductivity."

The work is published online in the journal *Nano Letters*. The paper was authored by Agrawal, Peng, Gdoutos and Espinosa, all from the McCormick School of Engineering and Applied Science at Northwestern University.

Source: Northwestern University

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