

Nanowires exhibit giant piezoelectricity

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Gallium nitride (GaN) and zinc oxide (ZnO) are among the most technologically relevant semiconducting materials. Gallium nitride is ubiquitous today in optoelectronic elements such as blue lasers (hence the blue-ray disc) and light-emitting-diodes (LEDs); zinc oxide also finds many uses in optoelectronics and sensors.

In the past few years, though, nanostructures made of these materials have shown a plethora of potential functionalities, ranging from single-nanowire lasers and LEDs to more complex devices such as resonators and, more recently, nanogenerators that convert [mechanical energy](#) from the environment (body movements, for example) to power electronic devices. The latter application relies on the fact that GaN and ZnO are also piezoelectric materials, meaning that they produce electric charges as they are deformed.

In a paper published online in the journal [Nano Letters](#), Horacio Espinosa, the James N. and Nancy J. Farley Professor in Manufacturing and Entrepreneurship at the McCormick School of Engineering and Applied Science at Northwestern University, and Ravi Agrawal, a graduate student in Espinosa's lab, reported that piezoelectricity in GaN and ZnO nanowires is in fact enhanced by as much as two orders of magnitude as the diameter of the nanowires decrease.

"This finding is very exciting because it suggests that constructing nanogenerators, sensors and other devices from smaller nanowires will greatly improve their output and sensitivity," Espinosa said.

"We used a computational method called Density Functional Theory (DFT) to model GaN and ZnO nanowires of diameters ranging from 0.6 [nanometers](#) to 2.4 nanometers," Agrawal said. The [computational method](#) is able to predict the electronic distribution of the nanowires as they are deformed and, therefore, allows calculating their piezoelectric coefficients.

The researchers' results show that the piezoelectric coefficient in 2.4 nanometer-diameter nanowires is about 20 times larger and about 100 times larger for ZnO and GaN nanowires, respectively, when compared to the coefficient of the materials at the macroscale. This confirms previous computational findings on ZnO nanostructures that showed a similar increase in piezoelectric properties. However, calculations for [piezoelectricity](#) of GaN nanowires as a function of size were carried out in this work for the first time, and the results are clearly more promising as GaN shows a more prominent increase.

"Our calculations reveal that the increase in piezoelectric coefficient is a result of the redistribution of electrons in the nanowire surface, which leads to an increase in the strain-dependent polarization with respect to the bulk materials," Espinosa said.

The findings by Espinosa and Agrawal may have important implications for the field of [energy harvesting](#) as well as for fundamental science. For energy harvesting, where piezoelectric elements are used to convert mechanical to electrical energy in order to power electronic devices, these results point to an advantage in reducing the size of the piezoelectric elements down to the nanometer scale. Energy harvesting devices built from small-diameter nanowires should in principle be able to produce more electrical energy from the same amount of mechanical energy than their bulk counterparts.

In terms of fundamental science, these results further previous

conclusions that matter at the nanoscale has different properties. It is clear now that by tailoring the size of nanostructures, their mechanical, electrical and thermal properties can be tuned as well.

"Our focus remains on understanding the fundamental principles governing the behavior of nanostructures as a function of their size," Espinosa and Agrawal say. "One of the most important issues that needs to be addressed is to obtain experimental confirmation of these results, and establish up to what size the giant piezoelectric effects remain significant."

Espinosa and Agrawal hope their work will spur new interest in the electromechanical properties of nanostructures, both from theoretical and experimental standpoints, in order to clear the path for the design and optimization of future nanoscale devices.

Provided by Northwestern University

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