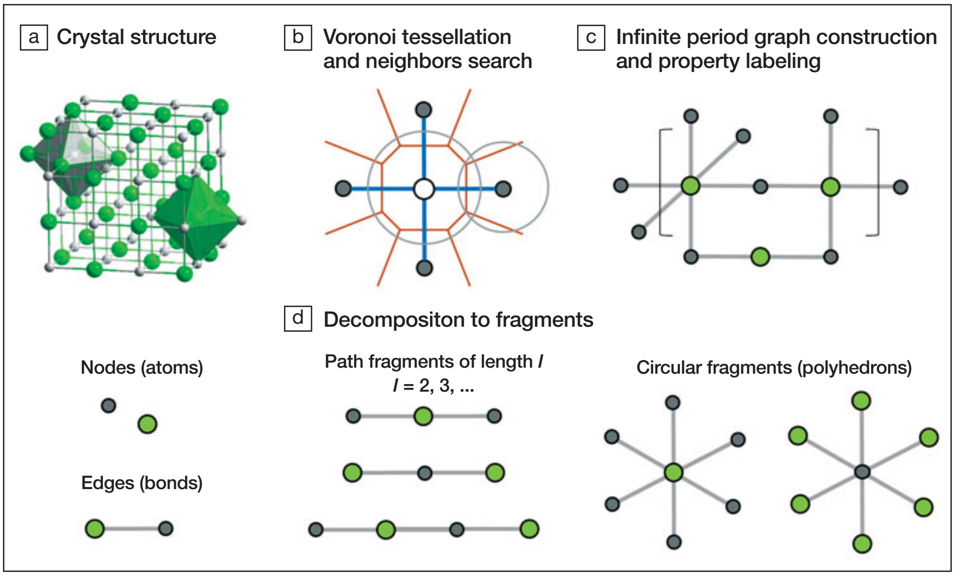
groups. Four of these groups are subjected to machine learning techniques to learn the best relationship or a "rule" that will predict a set of properties (e.g., Debye temperature, metal/nonmetal, and specific heat) from the corresponding fingerprint. This rule is tested on the fifth group to see how well the predictions match the observations. By rotating the five groups, all data get to be in the training set and the testing set.



In property-labeled materials fragments, the crystal structure (a) is analyzed for atomic neighbors through Voronoi tessellation (b). After property labeling, the resulting periodic graph (c) is decomposed into simple subgraphs (d). Credit: *Nature Communications*.

PLMF was tested on eight predictive models: a binary classification model to predict if a material is metal or nonmetal and seven regression models that predict the band energy, bulk and shear modulus, Debye temperature, heat capacities, and coefficient of thermal expansion. What distinguishes the team's work from other machine learning approaches is the high accuracy of these predictions. For example, the values for bulk and shear modulus are 99% accurate for the data set. The metal/nonmetal classification is 86% accurate for a sample set of 26,674 materials. In other words, only 3621 materials were misclassified in this case.

Keith Butler of the University of Bath complimented the team on the novel fingerprint technique: "The work of Isayev et al. presents one of the most convincing approaches for turning the structure and composition of a crystal into a form that is sensible to a machine learning algorithm. It's a big advance and it opens the door for future applications of machine learning for materials design."

Johannes Hachmann of the University at Buffalo, The State University of New York concurs: "One of the key challenges to making machine learning a viable proposition in this application domain is the availability of a suitable numerical representation of compounds in materials space. The proposed universal fragment descriptors offer an exciting new direction on this issue and promise to support easier interpretation of the resulting models and rational design based on these insights."

The research team plans to continue developing better algorithms and perhaps a unified model that will one day work for any materials system.

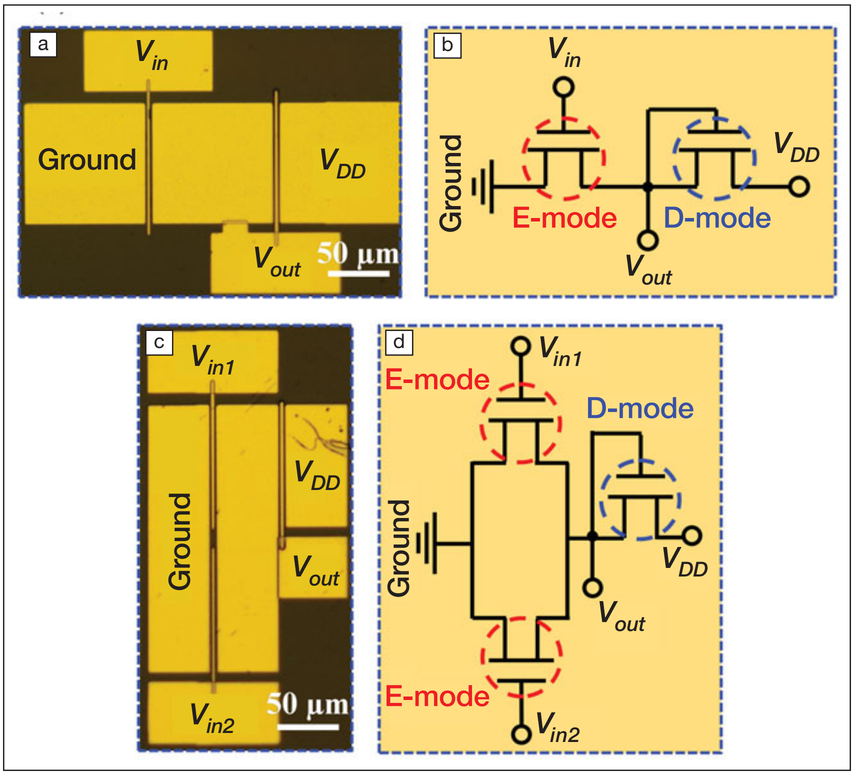
Vineet Venugopal

Diamond-powered transistor performs in extreme environments

Research is being conducted to employ wide-bandgap semiconductors such as SiC, GaN, and diamond to replace silicon to overcome its inherent limitations of high-frequency switching and power handling. Now researchers at the National Institute for Materials Science (NIMS) in Japan have designed a diamond-powered transistor that can be used in extreme environmental conditions like harsh temperatures and radiation conditions, as reported in a recent issue of *IEEE Electron Device Letters* (doi:10.1109/LED.2017.2702744). Due to their high power frequency, thermal limits, and low power loss at high frequency, diamond-based electronic devices outshine other wide-bandgap semiconducting materials-based devices.

In this study, the researchers used a microwave plasma-enhanced chemical vapor deposition technique to grow a 150-nm-thick epitaxial layer of hydrogenated diamond (H-diamond) at 900–940°C with a chamber pressure of 80 Torr. A 4-nm-thick layer of Al_2O_3 was selected as a buffer (to reduce the effect of lattice mismatch) for the $LaAlO_3$ to utilize H-diamond in enhancement-mode metal oxide semiconductor field-effect transistor (MOSFET) architecture, and a 30.4-nm-thick layer of Al_2O_3 was deposited on H-diamond for the operation of depletion-mode MOSFETs. Both types of devices were completed with Ti/Au metal deposition through e-beam evaporation. The schematic diagram of both circuits is shown in the Figure.

An increase in gain maximum for the NOT logic circuit from 1.2 to 26.1 was recorded when the voltage supplied was changed from –5.0 to –25.0 V. The NOR logic circuit configuration showed immaculate NOR gate characteristics.



Top views (a,c) and schematic diagrams (b,d) of the H-diamond metal oxide semiconductor field-effect transistor NOT and NOR logic circuits, respectively. The V_{in}, V_{out}, and V_{DD} represent input voltage, output voltage, and supply voltage, respectively. The V_{in1} and V_{in2} represent two input voltages for the NOR logic circuits. E-mode is enhancement mode and D-mode is depletion mode. Credit: *IEEE Electron Device Letters*.

According to Jiangwei Liu of NIMS, "The fabrication of logic circuits will push forward the development of diamond MOSFET current switches and digital circuits for high-temperature, high-power, high-frequency, energy-saving, and low-carbon practical applications."

"Enhancement mode (normally-off) is useful for diamond FET," says Hiroshi Kawarada from Waseda University. According to Kawarada, the research team should move toward high-temperature operation and record the radiation hardness of circuits. He adds, "It is really useful for the safe dismantling of nuclear reactors and taking out the debris." Yasuo Koide, vice president at NIMS, anticipates that these diamond-powered transistors will be commercialized for general applications in about 10 years. "However, in the limited field of radiation in the nuclear plant and space applications, the devices will be commercialized within five years," Koide says.

Liu believes that this is just the beginning and he would like to take his research in the direction of stable devices even at high temperatures. Currently, the diamond-based devices do not perform well if the operating temperature is above 300°C. He says, "The final target of my study is that the H-diamond-based devices such as NOR, NOT, NAND, and the ring oscillator can operate stably at more than 500°C." The roadmap for these advancements, he says, are "(a) to change the fabrication process, (b) to find a good ohmic contact metal to H-diamond, (c) to treat the H-diamond surface using plasma, and (d) to change the deposition conditions for the oxide insulator."

Rahim Munir