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Theory reveals the nature of crystals defects (of silicon carbide)

Imperfections of crystal structure, especially edge dislocations of an elongated nature, deeply modify basic properties of the entire material and, in consequence, drastically limit its applications. Using silicon carbide as an example, physicists from Cracow and Warsaw have shown that even such computationally demanding defects can be successfully examined with atomic accuracy by means of a cleverly constructed, small in size, model.

Mathematics loves perfection. Unfortunately, perfection does not love physical reality. Theoreticians modelling crystals have long tried to include defects in real crystalline structures and predict their impact on the physical properties of materials. The models, based on the results of various experiments, have described changes in the basic properties of a material without explaining the real causes and effects of the occurring phenomena.

A new model of silicon carbide (SiC), built by physicists from the Institute of Nuclear Physics of the Polish Academy of Sciences (IFJ PAN) in Cracow, has allowed them to demonstrate that now it is possible to study crystals *ab initio* with such complex defects as edge dislocations and to explain their characteristics by processes occurring on an atomic scale. This spectacular result, recently presented at the Multiscale Phenomena in Molecular Matter 2019 conference in Cracow, was achieved by the IFJ PAN physicists in cooperation with the Institute of Fundamental Technological Research of the Polish Academy of Sciences and the Institute of High Pressure Physics of the Polish Academy of Sciences, both located in Warsaw.

“We tried to find the mechanisms responsible at the atomic level for lowering the breakdown voltage in silicon carbide crystals. Our *ab initio* calculations lead to a qualitative understanding of the problem and contribute to explaining the details of this phenomenon”, says Dr. Jan Łażewski, professor at the IFJ PAN.

Ab initio calculations have now a long history related to Nobel Prize for Walter Kohn and John Pople in 1998 (however to linear crystal defect simulations they have only recently been introduced). This term is used to describe calculations carried out using quantum mechanics equations, supported only by knowledge about the structure of the atom and the symmetry of crystals. There is no direct information from experiments in such models, which means that they can also be used to analyse materials that have never been studied or even synthesized before. Because of relatively substantial complication of the issue, so far *ab initio* calculations worked, at most, in the case of point defects, related to vacancies (missing atoms or holes in the crystal structure) as well as admixtures introduced into the crystal.

It was not without reason that the Cracow researchers used silicon carbide. The properties of this semiconductor are so interesting that in the past it was even considered a successor to silicon. Its band gap (the barrier the charge has to overcome to get from the valence band to the conduction band and conduct current) is almost three times greater than in silicon, the permissible conduction current density – twice as great, the ability to dissipate heat – more than three times greater, and

the cutoff frequency of crystal operation as many as six times greater. In addition, silicon carbide systems can operate at temperatures up to 650 degrees Celsius, while silicon systems already begin to have problems at 120 degrees Celsius. SiC also has a high melting point, it is hard, resistant to acid and radiation. Its disadvantages include above all the price: whilst two-inch silicon wafers cost only a few dollars, the value of similar silicon carbide wafers runs into thousands. Low quality silicon carbide crystals are a popular abrasive material, also used in bulletproof vests and in the brake discs of the world's most expensive cars, such as Lamborghini or Bugatti. High quality crystals are used to produce mirrors for telescopes and in high voltage devices with high resistance to temperature.

At the atomic level, silicon carbide crystals are composed of many flat layers arranged one on top of each other. Each layer resembles a honeycomb: it consists of hexagonal cells in which the silicon carbide molecules are located vertically in the corners. Each two adjacent layers can be combined in three ways. The multilayer 'sandwiches' with different layouts create so-called polytypes, of which there exist more than 250 in the case of silicon carbide. The group from IFJ PAN used the 4H-SiC polymorph.

"When modelling such structures, one of the main problems is computational complexity. A model of pure crystal, devoid of admixtures or dislocations, is characterized by high symmetry and can be calculated even in a few minutes. In order to carry out a calculation for a material with dislocation, we need months working on a high power computer", emphasizes Dr. Paweł Jochym, professor at the IFJ PAN.

The problems with edge dislocations result from the scale of their influence on the crystal structure of the material. As an illustration, they can be compared to the problem of disguising a gap in a row of tiles on a floor. The gap can be 'camouflaged' by moving the tiles of adjacent rows, but the defect will always remain visible. Edge dislocations resulting from the lack of whole lengths or regions of atoms/molecules in individual crystal layers act similarly, affecting the positions of atoms and molecules in many adjacent layers. And since the dislocations can extend over long distances, in practice the disturbances caused by them include the entire crystal.

The most interesting phenomena take place in the dislocation core, i.e. in the vicinity of the edge of the damaged layer of the crystal network. In order to eliminate long-range effects caused by a single dislocation, and thus significantly reduce the number of atoms under consideration, a trick was employed: a second dislocation of the opposite effect was introduced. In this way, the impact of the first dislocation over longer distances was compensated for.

The SiC crystal model consisted of about 400 atoms. The simulations showed that in the layers of crystals, along the edge of the core of the defect, 'tunnels' appear in the form of channels with reduced charge density. They lower the potential barrier locally and cause electric charges to 'leak' from the valence band. In addition, in the forbidden gap, which in the insulator guarantees a lack of electrical conductivity, conditions appear which reduce its width and effectiveness in limiting the flow of charge. It was shown that these states originate from atoms located in the dislocation core.

"The situation can be compared to a deep, steep ravine that a squirrel is trying to cross. If the bottom of the ravine is empty, the squirrel will not get to the other side. However, if there are a number of trees at the bottom that are high enough, the squirrel can jump over their tops to the other side of the ravine. In the crystal we modelled, the squirrels are the electrical charges, the valence band is one edge of the ravine, the conduction band is the other, and the trees are the aforementioned states associated with the atoms of the dislocation core," says Prof. Łazewski.

Now that the mechanisms responsible for lowering the threshold of the energy barrier have become known at the atomic level, there is a huge scope for experimentation. The proposed mechanism will have to be verified in order to be able to use it to limit the negative influence of the tested defects. Fortunately, there are already technical possibilities for this.

"The future will verify whether our ideas will be confirmed in their entirety. However, we are confident about the fate of our model and the presented approach to simulating edge dislocations. We already know that the *ab initio* model has proved its worth in confrontation with certain experimental data", concludes Prof. Jochym.

The Henryk Niewodniczański Institute of Nuclear Physics (IFJ PAN) is currently the largest research institute of the Polish Academy of Sciences. The broad range of studies and activities of IFJ PAN includes basic and applied research, ranging from particle physics and astrophysics, through hadron physics, high-, medium-, and low-energy nuclear physics, condensed matter physics (including materials engineering), to various applications of methods of nuclear physics in interdisciplinary research, covering medical physics, dosimetry, radiation and environmental biology, environmental protection, and other related disciplines. The average yearly yield of the IFJ PAN encompasses more than 600 scientific papers in the Journal Citation Reports published by the Thomson Reuters. The part of the Institute is the Cyclotron Centre Bronowice (CCB) which is an infrastructure, unique in Central Europe, to serve as a clinical and research centre in the area of medical and nuclear physics. IFJ PAN is a member of the Marian Smoluchowski Kraków Research Consortium: "Matter-Energy-Future" which possesses the status of a Leading National Research Centre (KNOW) in physics for the years 2012-2017. The Institute is of A+ Category (leading level in Poland) in the field of sciences and engineering.

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SCIENTIFIC PAPERS:

1. "Destructive influence of the edge dislocation on 4H-SiC properties – DFT study"
J. Łażewski, P. T. Jochym, P. Piekarz, M. Sternik, K. Parliński
https://indico.ifj.edu.pl/event/212/attachments/1120/1642/BoA_Multis2019.pdf
2. "DFT modelling of the edge dislocation in 4H-SiC"
J. Łażewski, P. T. Jochym, P. Piekarz, M. Sternik, K. Parliński, J. Cholewiński, P. Dłużewski, S. Krukowski
Journal of Materials Science (2019) 54:10737-10745
DOI: 10.1007/s10853-019-03630-5

LINKS:

<https://multis2019.ifj.edu.pl/>

The website of the Multiscale Phenomena in Molecular Matter 2019 conference.

<http://www.ifj.edu.pl/>

The website of the Institute of Nuclear Physics Polish Academy of Sciences.

<http://press.ifj.edu.pl/>

Press releases of the Institute of Nuclear Physics Polish Academy of Sciences.

IMAGES:

IFJ190829b_fot01s.jpg

HR: http://press.ifj.edu.pl/news/2019/08/29/IFJ190829b_fot01.jpg

Silicon carbide crystal model with edge dislocations introduced in places marked in red. A single crystallographic plane is presented at the bottom. The places where electric charges can 'leak' to neighboring layers are marked in yellow. (Source: IFJ PAN)