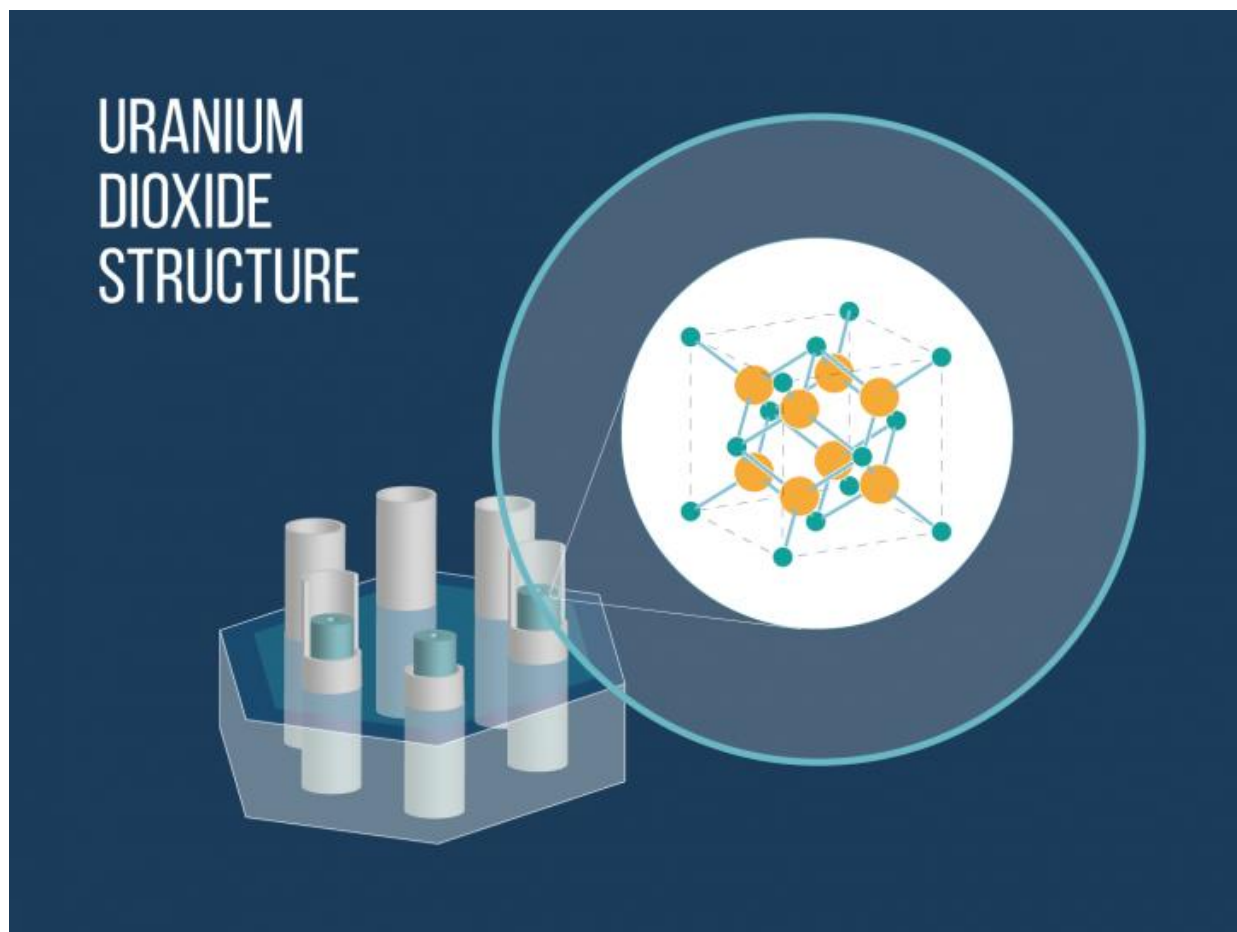


Researchers describe the mobility of line defects in uranium dioxide

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Uranium dioxide structure is illustrated. Credit: MIPT

Physicists from the Russian Academy of Sciences have described the

mobility of line defects, or dislocations, in uranium dioxide. This will enable future predictions of nuclear fuel behavior under operating conditions. The research findings were published in the *International Journal of Plasticity*.

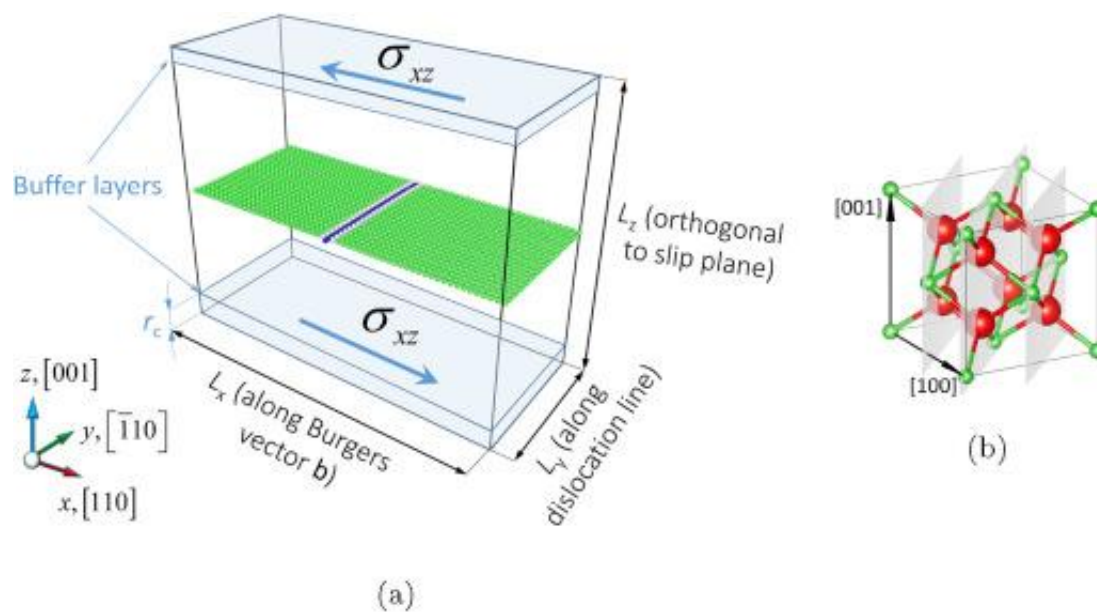
Nuclear fuel has immense potential, as it is one of the most energy-dense resources available—a single [uranium dioxide](#) fuel pellet weighing no more than a few grams releases the same amount of energy within the reactor core that is produced by burning several hundred kilograms of anthracite coal or oil. When a nuclear reactor is in operation, the fuel in the pellets undergoes extremely complex transformations caused by both temperature and radiation. Because the underlying mechanisms of these transformations are not yet fully understood, we are still unable to realize the complete potential of nuclear fuel and reduce the risk of accidents to a minimum.

The mechanical properties of fuel pellets, which play an important part in nuclear engineering, are determined by the motion and interaction of dislocations. Dislocation mobility in uranium dioxide at [high temperatures](#) and under stress has never been studied in detail. Now, recent research into dislocation dynamics has been carried out by Artem Lunev, Alexey Kuksin, and Sergey Starikov. In their paper, the scientists report on a simulation of dislocation behavior in uranium dioxide, which is one of the most widespread compounds used as nuclear fuel on power plants across the globe.

To be used as nuclear fuel, uranium dioxide is formed into ceramic pellets that are sintered at a high temperature. This material has a very high melting point, is resistant to radiation-induced growth, and does not experience phase transitions within a broad temperature range.

Theoretically, a solid body has a regular, ordered structure (crystalline structure), and there is a certain designated position for each atom to occupy. In reality, perfect crystals do not exist, because some atoms or

groups of atoms are always out of place, altering the ideal arrangement. In other words, there are defects (imperfections) in an actual crystal. They come in several types, viz., point defects, line defects (dislocations), planar defects and bulk defects. Defects can move within the crystal, and the nature of their motion depends on external factors. Dislocation dynamics are known to determine fuel properties relevant to nuclear engineering (plasticity, fission fragments diffusion).



This image shows: (a) Simulation setup for studying dislocation dynamics in a uranium dioxide crystal under applied shear stress σ_{xz} . Uranium atoms on lattice points of the perfect uranium sublattice within the uranium oxide crystal are shown in green. The line defect that corresponds to a distortion of the perfect crystal lattice is shown in blue. (b) The perfect uranium dioxide crystal structure with the green and red spheres representing uranium and oxygen atoms respectively. Credit: MIPT Press Office

In their study, the scientists from MIPT and the Joint Institute for High Temperatures used computational methods to develop a model of an

isolated dislocation in a perfect uranium dioxide crystal. They calculated the varying dislocation velocity as a function of temperature and the external forces affecting the crystal.

The researchers analyzed simulation results within the framework of statistical physics and obtained a model that describes the behavior of dislocations in a broad temperature range under shear stress of various magnitudes. This model enables the calculation of dislocation velocity based on the known temperature and stress parameters.

The model proposed by the Russian scientists could soon be used to simulate more complex systems and study the macroscopic processes occurring in [fuel pellets](#) under operating conditions.

"This is a major advance toward describing processes as complex as nuclear fuel swelling and embrittlement during operation by means of computer simulations alone," says Sergey Starikov, a coauthor of the study, an associate professor at MIPT, and a senior researcher at the Joint Institute for High Temperatures.

Computer modeling enables scientists to trace individual fuel atoms and calculate their velocities and the forces affecting them, along with other parameters. This allows systems of various complex configurations to be simulated and studied. Computer modeling is widely used in situations where performing an experiment is problematic. Research into [nuclear fuel](#) behavior is one of those areas. Such large-scale calculations rely on modern supercomputers, as massive computing power is required to find the forces affecting individual atoms at each moment in time.

More information: A.V. Lunev et al, Glide mobility of the $1/2[1\ 1\ 0](0\ 0\ 1)$ edge dislocation in UO_2 from molecular dynamics simulation, *International Journal of Plasticity* (2016). [DOI: 10.1016/j.ijplas.2016.11.004](#)

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