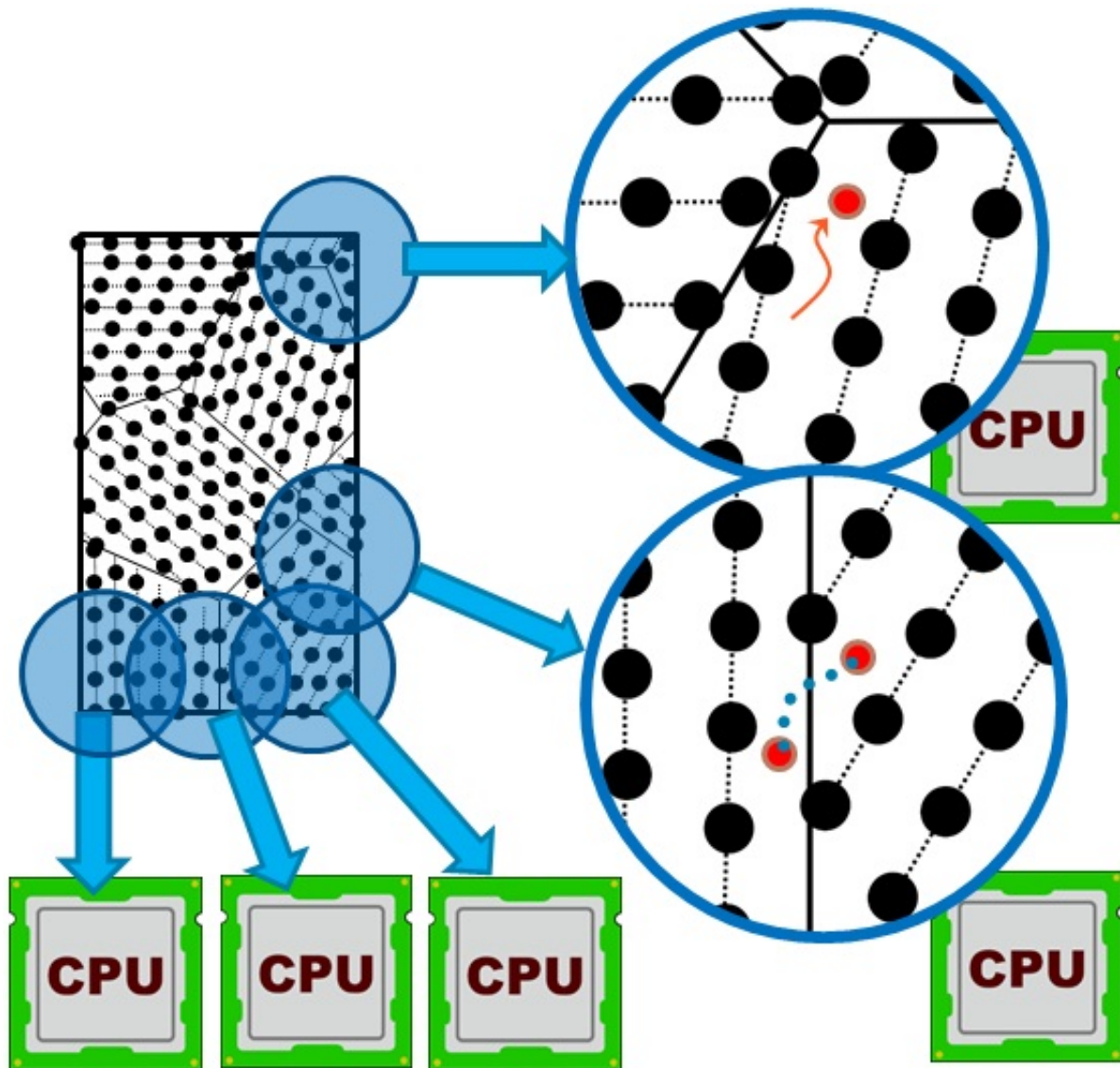


How do impurities move in tungsten?

June 30 2017



The calculation of each small domain has been input as an independent task in each CPU of the supercomputer. By integrating those results we find the migration path in the whole material. The image of the CPU in the image is copyrighted and is used from avaxhome.ws. Credit: Dr. Atsushi M. Ito

One part of the vacuum vessel (the plasma facing material) of the fusion experimental device and future fusion reactor comes into contact with plasma. When the plasma ions enter into the material, those particles become a neutral atom and stay inside the material. If seen from the atoms that compose the material, the plasma ions that entered become impurity atoms. The impurity atoms migrate slowly in interspaces among the atoms that composes the material and eventually, they diffuse inside the material. On the other hand, some impurity atoms return to the surface and are again emitted to the plasma. For the stable confinement of fusion plasma, the balance between the penetration of plasma ions into the material and the re-emission of impurity atoms after migration from inside the material becomes extremely important.

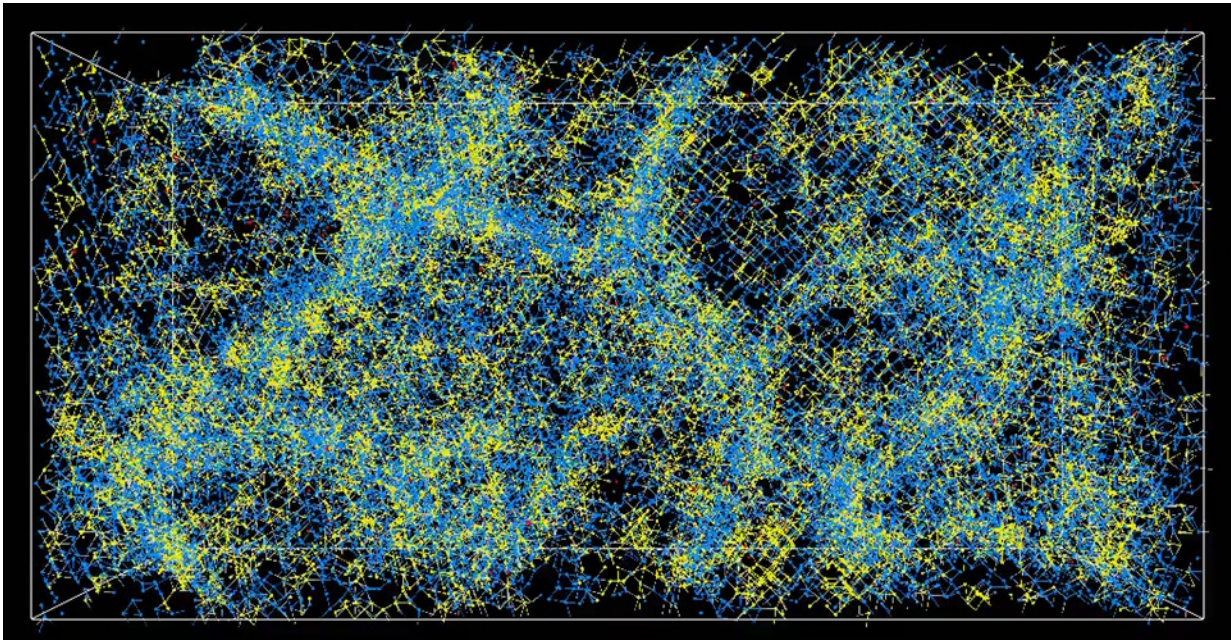
The migration path of impurity [atoms](#) inside materials with ideal crystal structure has been well elucidated in many research. However, actual materials have polycrystalline structures, and then migration paths in grain boundary regions had not been clarified yet. Further, in a material that continuously touches plasma, the crystal structure is broken due to the excessive incursion of plasma ions. The migration paths of impurity atoms inside a material with a disordered crystal structure had not been sufficiently examined.

The research group of Professor Atsushi Ito, of National Institutes of Natural Sciences NIFS, has succeeded in developing a method for automatic and rapid search regarding migration paths in materials having arbitrary atom geometry through molecular dynamics and parallel calculations in a supercomputer. First, they take out numerous number of small domains that cover the entire material.

Inside each small domain they compute the migration paths of impurity atoms through molecular dynamics. Those calculations of small domains

will be finished in a short time because the size of the domain is small and the number of atoms to be treated is not many. Because the calculations in each small domain can be conducted independently, calculations are performed in parallel using the NIFS supercomputer, the Plasma Simulator, and the HELIOS supercomputer system at the Computational Simulation Centre of International Fusion Energy Research Centre (IFERC-CSC), Aomori, Japan. On the Plasma Simulator, because it is possible to use 70,000 CPU cores, simultaneous calculations over 70,000 domains can be performed. Combining all of the calculation results from the small domains, the migration paths over the whole material are obtained.

Such a parallelization method of super computer differs from the one often used, and is called MPMD3)-type parallelization. At NIFS, a simulation method that effectively uses MPMD-type parallelization had been proposed. By combining the parallelization with recent ideas regarding automatization, they have arrived at a high-speed automatic search method for the migration path.



The simulation result is based upon the dynamic Monte Carlo method⁴). Inside the base material of the tungsten, the atoms of which structure is close to the crystal are not displayed, and the tungsten atoms near the crystal grain boundary, which are of out-of-crystal deformation, are displayed as yellow and blue-colored points. The tracks of the impurity atoms moving inside (in this example, helium atoms) are displayed in white. So to make the impurities moving at high speed visible to the human eye, in order to indicate the tracks of the impurity atoms we have made all tracks resemble a tail with a fixed length, and we are seeking to express that movement of clouds as "averaged behavior." Credit: Dr. Atsushi M. Ito

By utilizing this method, it becomes possible to search easily the migration path of impurity atoms for actual materials that have crystal grain boundaries or even [materials](#) of which [crystal structure](#) become disordered by long duration contact with plasma. Investigating the behavior of collective migration of [impurity atoms](#) inside material based upon information regarding this [migration](#) path, we can deepen our knowledge regarding the particle balance inside the [plasma](#) and the material. Thus improvements in [plasma confinement](#) are anticipated.

These results were presented in May 2016 at the 22nd International Conference on Plasma Surface Interaction (PSI 22), and will be published in the journal *Nuclear Materials and Energy*.

More information: Atsushi M. Ito et al, Automatic kinetic Monte-Carlo modeling for impurity atom diffusion in grain boundary structure of tungsten material, *Nuclear Materials and Energy* (2017). [DOI: 10.1016/j.nme.2017.04.010](#)

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