Molecular dynamics simulations of interactions with various materials starting with plasma-wall interaction studies

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1. Plasma-wall interaction

In a fusion plasma device, it is necessary to confine high-temperature plasma in a vacuum vessel. In this process, the plasma is designed to come into contact a component called the divertor plate, which minimizes dissolution heating of the vessel. We used molecular dynamics (MD) simulation to study plasma irradiation-induced damage to divertor plates (see Figure 1). Here, the plasma-wall interaction (PWI) is calculated by MD for elementary processes. This simulation was our first application of the MD method to fusion research[1-6].

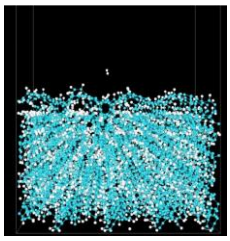

Figure 1 Hydrogen molecule from graphite wall[3].

2. DNA double-strand break

In recent years, starting with this PWI research, we have expanded the scope of application beyond divertor plates. In the MD method, the motion trajectory of many particles can be obtained by numerically integrating the classical equation of motion.

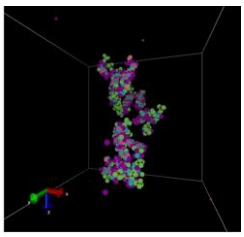

Figure 2 Snapshot of DNA double-strand breaks

Taking advantage of this feature, we quantitatively evaluated the effects of tritium on biomolecules (DNA). Tritium, a radioactive isotope of hydrogen, which is the fuel of the nuclear fusion reactor, emits β-rays. External exposure is not a problem, only internal exposure caused by taking tritium into the body needs to be controlled.
In order for fusion power generation to be accepted by society, it is necessary to accumulate scientific knowledge that will enable a rigorous assessment of the risks of tritium[7,8]. Therefore, we evaluated tritium-induced DNA damage by MD[9] as shown in Figure 2.

3. Chiral nanoneedle by optical vortex

The third topic is electromagnetic fields, which are often used to heat fusion plasmas. As this electromagnetic field, we consider an optical vortex, which is an electromagnetic wave with orbital angular momentum. It is known that when a metal is irradiated with an optical vortex, the surface of the material melts into a helical nanostructure[10], and we have successfully created this structure on a computer using MD (Figure 3). We introduce this structure formation obtained by MD simulation[11].

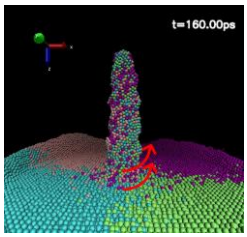

Figure 3 Structure formation of chiral nanoneedle[11]

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