3. Numerical Simulation Reactor Research Project

Fusion plasmas are complex systems which involve a variety of physical processes interacting with each other across wide ranges of spatiotemporal scales. In the National Institute for Fusion Science (NIFS), we are utilizing the full capability of the supercomputer, Plasma Simulator (Fig.1), and propelling domestic and international collaborations in order to conduct the Numerical Simulation Reactor Research Project (NSRP). Missions of the NSRP are i) to systematize understandings of physical mechanisms in fusion plasmas for making fusion science a well-established discipline and ii) to construct the Numerical Helical Test Reactor, which is an integrated system of simulation codes to predict behaviors of fusion plasmas over the whole machine range.

Presented below in Figs. 2 and 3 are examples of successful results from collaborative simulation researches in 2018–2019 on kinetic ballooning mode (KBM) turbulence and on generation of helical structures in a reversed field pinch (RFP) plasma. Also, highlighted in the following pages are achievements of the NSRP on plasma fluid equilibrium stability, energetic-particle physics, neoclassical and turbulent transport simulation, integrated transport simulation, and plasma-wall interaction.

(H. Sugama)



Fig. 1 The Plasma Simulator, PRIMEHPC FX100.



Fig. 2 Electrostatic potential fluctuations obtained by global gyrokinetic simulation of kinetic ballooning mode (KBM) turbulence in a tokamak plasma [presented by A. Ishizawa (Kyoto University)].



Fig. 3 Pressure of a reversed field pinch (RFP) plasma obtained by nonlinear MHD simulation [presented by collaboration of N. Mizuguchi (NIFS) and Kyoto Institute of Technology]. Generation of helical structures in the RFP plasma is clarified.

Numerical and theoretical MHD studies for Heliotron plasmas

Highlight

Numerical analysis of MHD instabilities based on kinetic MHD model with kinetic effects of thermal ions

For the inward shifted LHD configurations, where the magnetic axis is shifted inward relative to the center of helical coils, the MHD stability was considered to be unfavorable since there is always a magnetic hill. However, high beta plasmas with β ~5% have been experimentally established in the inward shifted LHD configurations where β is the volume averaged beta value. It is a crucial issue to clarify the mechanism how such high beta plasmas are obtained. In this study, we have extended the numerical model such that the kinetic effects of thermal ions are taken into account, i.e., kinetic MHD model, and the kinetic effects of the thermal ions on resistive ballooning modes in high beta LHD plasmas have been investigated. From the numerical analysis based on the kinetic MHD model, it is found that the kinetic effects reduce the linear growth rate of pressure driven MHD instabilities. Figure 1 shows the trajectory of a deeply trapped ion and the image map of the perturbed electron pressure due to the resistive ballooning mode on a magnetic surface where the red and the blue correspond to the positive amplitude and the negative amplitude, respectively. The trapped ion has the precession motion in both poloidal and toroidal directions. When the precession drift frequency of the trapped ions with respect to the mode phase is close to or larger than the linear growth rate of the instability, the response of the trapped ions is weakened. This results in the suppression of the ion perpendicular pressure perturbation to the magnetic field leading to the reduction of the linear growth rate.

[1] M. Sato and Y. Todo, Proc. IAEA FEC 2018 (Ahmedabad, India), TH/P5-25.



Fig. 1 The trajectory of a deeply trapped ion and the image map of the perturbed electron pressure due to the resistive ballooning modes on a magnetic surface. Here the red and the blue correspond to the positive and the negative amplitude, respectively.

Toroidal MHD equilibrium calculation via simulated annealing

We have demonstrated that simulated annealing (SA), a new method to calculate equilibria of ideal fluids, successfully achieves toroidal equilibria of tokamak and toroidally-averaged heliotron plasmas. The SA is a kind of relaxation theory that utilizes the Hamiltonian nature of the ideal fluids, including MHD. By solving an initial-value problem of an artificial dynamics derived on the basis of the Hamiltonian and the Poisson bracket. If the system is described by noncanonical variables, the Poisson bracket has null spaces called Casimir invariants. The artificial dynamics of the SA is constructed so that the energy of the system changes monotonically while the Casimir invariants are preserved. The system asymptotically approaches an energy extremum that is an equilibrium. In this study, we have extended the previous studies using low-beta reduced MHD model for cylindrical plasmas, and have suc-

ceeded to calculate large-aspect-ratio and circular crosssection equilibria of tokamak and toroidally-averaged heliotron plasmas by using high-beta reduced MHD model. For the toroidally-averaged heliotron plasmas, we have compared our numerical results for Heliotron E by the STEP-EQ code. In Fig. 2, the magnetic axis shift against the central beta value (Left) and flux surfaces on a poloidal cross-section (Right) are shown. Complete agreement is difficult to obtain mainly because the netcurrent-free condition cannot be imposed in the SA at present. However, we have obtained reasonable agreement with the previous results.

[1] M. Furukawa et al., Phys. Plasmas 25, 082506 (2018).



Fig. 2 Left: Magnetic axis shift increases as the central beta value is increased. Right: Flux surfaces are plotted for an equilibrium with central beta value 11%.

(M. Furukawa, Tottori University)

Numerical simulation of interaction between global flow and interchange modes in heliotron plasmas

In some special discharges in the Large Helical Device (LHD) experiments, partial collapses of the electron temperature profile due to the interchange mode are observed. In the collapses, the onset of the mode growth and the mode rotation stop are synchronized [1]. This phenomenon suggests the stabilizing contribution of the background flow on the interchange mode. Thus, we analyze the nonlinear evolution of the interchange mode with keeping the flow by means of three-dimensional (3D) simulations. For this purpose, we have developed the numerical scheme to calculate the 3D profile of the flow consistent with experimental data at first [2], which is observed in a one-dimensional direction in LHD [3]. A static equilibrium calculated with the HINT code [4] is utilized as the initial state in the nonlinear dynamics simulation with the MIPS code [5]. The 3D flow results are incorporated in the initial perturbation. We apply this procedure to a strongly unstable static equilibrium. As shown in Fig. 3, the pressure profile is deformed due to the interchanged mode in the no flow case. When we increase the flow up to the 10 times larger amount of that in the experiment, such deformation is reduced. However, when we apply 30 times larger flow, the Kelvin-Helmholtz instability appears and enhances the deformation again. Thus, the background flow can

provide the stabilizing window between the interchange and the Kelvin-Helmholtz instabilities.

- [1] S. Sakakibara et al., 2015 Nuclear Fusion 55, 083020.
- [2] K. Ichiguchi et al., Proc. IAEA FEC 2016 Kyoto, TH/ P1-4.
- [3] M. Yoshinuma *et al.*, Fusion Science Tech. **58**, 375 (2010).
- [4] Y. Suzuki et al., 2006 Nucl. Fusion 46, L19.
- [5] Y. Todo et al., 2010 Plasma and Fusion Res. 5, S2062.



Fig. 3 Total pressure profile at early nonlinear saturation phase for the cases with (a) no flow, (b) flow with 10 times larger amount of the experiment, and (c) flow with 30 times larger amount of the experiment. (K. Ichiguchi)

Energetic Particle Physics

Highlight

Ion heating by plasma oscillations is demonstrated by the state-of-the-art simulation

In the future fusion reactors, energetic alpha particles born from the deuterium-tritium fusion reaction are expected to heat the bulk plasma through collisions to sustain the high temperature needed for the fusion reaction. However, the bulk ion heating by the energetic alpha particles through collisions is weak, while the electron heating is dominant. If the ion heating efficiency is enhanced, this leads to the improvement of the performance of fusion reactor. A mechanism called "alpha channeling" where alpha particle energy is transferred to bulk ions through the interaction with plasma oscillations was proposed a long time ago but has not been demonstrated.

Energetic particle driven geodesic acoustic modes (EGAMs) are electrostatic plasma oscillations in toroidal plasmas. EGAMs in the Large Helical Device (LHD) plasmas were studied with hybrid simulations for energetic particles interacting with a magnetohydrodynamic (MHD) fluid [1,2]. Recently, the program was extended to simulate bulk ions as particles in addition to energetic particles [3]. This extension enables us to investigate the energy channeling from energetic particles to bulk ions. The extended simulation was applied to EGAMS in the LHD plasmas. The plasma pressure fluctuations of an EGAM in the simulation are shown in Fig. 1. It was demonstrated for the first time that the energetic particle energy is transferred to the

bulk ions through the interaction with the EGAM [4]. This result is expected to accelerate the studies of alpha channeling in experiment, theory, and simulation.



Fig. 1 Plasma oscillation excited by energetic particles in LHD. Plasma pressure fluctuations on the cross-sections of the doughnut-shaped plasma are shown in the figure. The red and green colors represent increase and decrease, respectively. The blue arrows indicate the time evolution.

- [1] H. Wang et al., Phys. Plasmas 22, 092507 (2015).
- [2] H. Wang et al., Phys. Rev. Lett. 120, 175001 (2018).
- [3] Y. Todo *et al.*, "A new magnetohydrodynamic hybrid simulation model with thermal and energetic ions", in ITC-26 and APFA-11 (Dec. 5-8, 2017, Toki, Japan).
- [4] H. Wang et al., Nucl. Fusion 59, 096041 (2019).

Critical energetic particle distribution in phase space for the Alfvén eigenmode burst with global resonance overlap

Comprehensive computer simulations of the Alfvén eigenmode burst, which is the synchronized sudden growth of multiple Alfvén eigenmodes interacting with energetic particles, were conducted with continuous neutral beam injection, collisions, and particle losses [5]. Figure 2 shows the amplitude evolution of multiple Alfvén eigenmodes and the evolution of energetic particle transport flux profile. It is found in the simulation result that the energetic-particle distribution in phase space reaches a "critical distribution" with a stairway structure where a resonance overlap triggers the Alfvén eigenmodes associated with the beam injection broadens the resonant regions in phase space forming the distribution into a stairway shape. When the distribution reaches the "critical distribution", a resonance overlap triggers multiple resonance overlaps leading to the synchronized growth of Alfvén eigenmodes and the collapse of the distribution. For another run with the beam deposition power reduced to one-half, the fast ion distribution function

just before the Alfvén eigenmode burst is close to that for the original beam power. This result indicates that the critical distribution for the Alfvén eigenmode burst is present.

[5] Y. Todo, Nucl. Fusion 59, 096048 (2019).

(Y. Todo)



Fig. 2 (a) Radial profile evolution of fast ion energy transport flux in the radially outward direction, and amplitude evolution of radial MHD velocity fluctuation for (b) the dominant n=2 (red) and n=3 (blue) Alfvén eigenmodes and (c) the other Alfvén eigenmodes with n=1-3. The unit of color bar is MW [5].

Energetic Ion Driven Instabilities near the Lower Hybrid Resonance Frequency

Using a one-dimensional electromagnetic particle code which simulates self-consistently the full ion and electron dynamics, we studied instabilities driven by energetic ions injected continuously in a plasma where the density



Fig. 3 Time variations of magnetic fluctuations in the frequency range of $0.5 < \omega/\Omega_i < 8$. The stair-like frequency chirping appears near the line $\omega = \omega_{LH}$ [6].

and the lower-hybrid resonance frequency ω_{LH} increase with time [6]. We show in Fig. 3 the amplitudes of all the waves in the frequency range $0.5 < \omega/\Omega_i < 8$, where Ω_i is the ion cyclotron frequency, the color indicates the amplitudes of the magnetic fluctuations, and the yellow line represents the frequency ω_{LH} . We see in Fig. 3 that the ion cyclotron harmonic wave with $\omega \approx l \Omega_i$, where l is an integer, is excited when ω_{LH} becomes close to $l\Omega_i$. When ω_{LH} is greater than $l\Omega_i$, this wave couples with the ion Bernstein mode that has the dispersion curve connecting to ω_{LH} . We also see in Fig. 3 that as a result of the instabilities and the wave-wave coupling, the stair-like frequency chirping with the riser Ω_i appears in the magnetic fluctuations in the frequency range of ω_{LH} . The frequency chirping has characteristics similar to the frequency chirping observed in the radio frequency radiations at the plasma start-up phase of the LHD experiments.

[6] M. Toida et al., Plasma Fusion. Res. 14, 3401112 (2019).

(M. Toida)

Study on the impurity transport phenomenon in LHD plasmas

Highlight

Global neoclassical transport simulation including the effect of small potential variation on the flux surfaces tackles with the unresolved problem of "impurity hole"

To realize steady-state operation of fusion reactor, accumulation of heavy impurity ions which come out from plasma-facing walls to the core plasma should be mitigated because they lead to radiation energy loss and decrease the performance of the plasma. From the conventional neoclassical transport theory, it is expected that the ambipolar radial electric field in $T_i \simeq T_e$ helical plasma is negative, which drags the impurity particle flux inward. Therefore, impurity accumulation is concerned in the future helical reactor. In LHD experiments, however, it was observed that impurity ions were sometimes expelled from the core region, although the neoclassical calculation predicted the negative electric field. Many theories and simulation studies have been trying to explain this "impurity hole phenomenon". One of possible extensions to the neoclassical transport simulation is to include the effect of electrostatic potential variation on the flux surface, which is caused by density anisotropy of bulk hydrogen ions. The potential variation, called " ϕ_1 potential", is usually as weak as $e\phi_1/T_e \sim 10^{-3}$, and its effect is negligible for bulk hydrogens and electrons. However, some preceding simulation studies have shown that the ϕ_1 potential substantially changes the impurity flux if the condition is set similar to the impurity hole plasma. Although the importance of ϕ_1 potential is recognized, no simulation studies so far have reproduced the outward impurity neoclassical flux to explain the impurity hole. However, the neoclassical transport simulation model can be further improved. FORTEC-3D code [1], which has been developed in NIFS, solves the global 5D drift-kinetic equation to evaluate the neoclassical transport. Since all the preceding ϕ_1 -effect studies are based on the radially-local approximation, extension of FORTEC-3D to include the ϕ_1 -effect is the world first challenge to study this problem using a global code. We have evaluated the ϕ_1 potential in an LHD plasma which is similar to the condition of impurity hole plasma and compared with local approximation simulations [2]. As shown in fig. 1, it is found that not only the amplitude but also the phase of the ϕ_1 potential is different between the radiallylocal and global simulation models. It is thought that the tangential magnetic drift, which is neglected in the



Fig. 1 Potential variation on a flux surface (r=0.6a) in an LHD plasma, calculated from a radially-local approximation (left) and global FORTEC-3D code (right). Here, (θ, ζ) represents the poloidal and toroidal angle [2].

S. Satake, Y. Idomura, H. Sugama *et al.*, Computer Phys. **181**, 1069 (2010).
K. Fujita, S. Satake *et al.*, Plasma Fusion Res. **14**, 3403102 (2019).

radially-local model, is actually comparable to the E × B drift by the radial electric field in impurity hole plasma, and it affects the hydrogen density and the ϕ_1 potential variation. This finding suggests that the local approximation model is insufficient to predict the impurity neoclassical flux including the ϕ_1 -effect. FORTEC-3D now is being upgraded for multispecies plasma, and the impurity flux in the global code will be calculated in the near future.

Reduced models for particle and heat transport by gyro-kinetic analysis with kinetic electron response

The particle and heat transport driven by the ion temperature gradient instability in helical plasmas is investigated by the gyrokinetic analysis taking into account the kinetic electron response [3]. Two types of transport models with a lower computational cost to reproduce the nonlinear gyrokinetic simulation results within allowable errors are presented for application in quick transport analyses. The turbulent electron and ion heat diffusivity models are given in terms of the linear growth rate and the characteristic quantity for the linear response of zonal flows, while the model of the effective particle diffusivity is not obtained for the flattened density profile observed in the LHD. The quasilinear flux model is also shown for the heat transport. The quasilinear flux models for the energy fluxes are found to reproduce the nonlinear simulation results at the accuracy similar to that of the heat diffusivity models. In addition, the quasilinear particle flux model, which is applicable to the transport analysis for LHD plasmas, is constructed and reproduces the nonlinear simulation results in the left of Fig.2. These turbulent reduced models enable coupling to the other simulation in the integrated codes for the LHD.

(S. Toda)

Temperature profile stiffness in turbulent transport of helical plasmas for flux-matching method

The plasma temperature profile sensitivities of the turbulent transport fluxes in helical plasmas are evaluated by the gyrokinetic simulations. Especially, in the simulations for the ion temperature gradient (ITG) turbulence in the LHD, it is found that the ion temperature gradients around the experimental observations are near the threshold of the instability, and the ion heat transport coefficients are quite sensitive to the temperature gradient. Using the statistical technique of Akaike's Information Criterion (AIC), a novel technique to determine the ranges of the temperature gradients possible given the experimentally obtained temperature data with errorbars is proposed. And the flux-matching method to predict the ion temperature gradient against the ranges of the temperature gradients is demonstrated for high ion temperature LHD plasma [4]. See the right of Fig.2. The results in the case of the simulations with adiabatic electron responses assumptions can predict the ion temperature gradient which agrees with the allowable temperature gradient ranges obtained from the AIC technique. On the other hand, in the simulations with kinetic electrons, the results are less than the adiabatic electron cases, because the simulations performed here are restricted under the assumptions that there are unintroduced effects such as ExB shearing effects, which may improve the predictions for ion heat transport, we should improve the simulation model.

[3] S. Toda et al., Phys. Plasmas 26, 012510 (2019).

[4] M. Nunami et al., Phys. Plasmas 25, 082504 (2018).



Fig. 2 Left: The comparison of the nonlinear simulation results for the particle flux with the quasi-linear flux model. Right: The allowable ranges of the temperature gradients evaluated by AIC technique (red curves) and the applications of the flux-matching method to expect the ion temperature gradients based on the simulations with kinetic electrons (blue diamond) and with adiabatic electrons (green circles).

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(M. Nunami)

Numerical Simulation Reactor Research Project

TASK3D-a

TASK3D-a, Integrated Transport Analysis Suite, Has Been Facilitating LHD Deuterium Experiment Analyses

Further extension has been made in TASK3D-a [1], in particular, for facilitating analyses of LHD deuterium plasmas, such as on NBI (neutral beam injection)-heating and neoclassical transport in the presence of multiple ions (including hydrogen and deuterium as main species), neutron emission rate, and behaviour of energetic particles. The applications of this extended TASK3D-a (as shown in Fig. 1) have provided systematic analyses datasets and experimental validations for important research topics of LHD deuterium experiment. Issue-resolutions related to its applications have been made by TASK3D-a developer(s), which has been also critical for TASK3D-a to be routinely applied to experiment analyses.



Fig. 1 Overview of extension of TASK3D-a series. Based on the first version, TASK3D-a01 released in 2012, several modules have been implemented (a02) and NBI module was upgraded (a03 and a04). Purple parts are related to analyses on the neoclassical transport in the presence of multiple ion species, neutron emission rate and energetic particles behaviour.

The integrated transport analysis suite, TASK3D-a [1], has been further extended mainly pursuing the increase of analyses capabilities of LHD deuterium experiments and of plasmas consisting of multiple ion species. The current overview of TASK3D-a suite is shown in Fig. 1. This extension includes extension of NBI heating analysis module in order to be applicable to the plasmas with hydrogen, deuterium and helium [2], and subsequent release of extended versions of TASK3D-a, such as TASK3D-a03 and -a04 as indicated in Fig. 1 (NBI module). This extension has been critical to provide systematic transport analyses database to investigate isotope effects in LHD deuterium experiments [3,4].

Programmatic actions have also been made for analyses of the neutron emission rate and the energetic particles behaviour. The database, created by employing the TASK3D-a framework for the neutron emission rate in a wide range of temperature and density [5], has been routinely utilized to machine time allocations. TASK/FP [6], which is the module of TASK [7] for solving the Fokker-Planck equation, has been implemented in TASK3D-a framework. It has greatly facilitated the energetic particles behaviour of LHD deuterium plasmas, such as analyses on distribution functions of beam energy in NBI-blip experiment [8], and validation calculations on nonlinear collision effects during the process of slowing down [6].

In this way, TASK3D-a has been extended by implementing new modules and upgrading the previously included modules, to be more relevant to experimental conditions. It has been routinely utilized as the integrated analyses framework for a variety of research topics.

An example of accumulated transport analyses database is shown in Fig. 3 [9] (this is only a tiny part of overall TASK3D-a analyses results), which has opened a linkage to so-called data-driven science. Some trials for modelling ion heat diffusivity [10,11] have been made based on statistical approach exploiting "largeness" of TASK3D-a analyses database. This is another aspect of the significance of TASK3D-a.

- [1] M. Yokoyama et al., Nucl. Fusion 57, 126016 (2017).
- [2] P. Vincenzi et al., Plasma Phys. Control. Fusion 58, 125008 (2016).
- [3] H. Yamada et al., 27th IAEA Fusion Energy Conference (FEC), EX/P3-5 (Ahmedabad, Oct. 2018).
- [4] K. Tanaka et al., 27th IAEA FEC, EX/P3-6 (Ahmedabad, Oct. 2018), submitted to Nucl. Fusion (2019).
- [5] R. Seki et al., accepted for publication in Plasma Fus. Res. (2019).
- [6] H. Nuga et al., Nucl. Fusion, 59, 016007 (2019).
- [7] A. Fukuyama, http://bpsi.nucleng.kyoto-u.ac.jp/task
- [8] H. Nuga et al., European Physics Society Conference 2017, P1.146 (Belfast, Jun. 2017).
- [9] M. Yokoyama, Plasma Fus. Res. 9, 1302137 (2014).
- [10] M. Yokoyama and H. Yamaguchi, Plasma Fus. Res. 14, 1303095 (2019).
- [11] M. Yokoyama, submitted to Nucl. Fusion (2019).



(fitted) [keV] (fitted) 0 0.4 0.6 0.4 0.6 ren/a99 0.8 (c (fitted) [10¹⁹ m⁻³] $\chi_{i,dynamic}$ [m²/s] ů 0 0.4 0.6 1^L 0.4 0.6 rett/200 0.8 02 0 8

Fig. 2 Sample of database of neutron emission rate for (upper) beam-bulk and (lower) bulk-bulk components. The color represents the neutron emission rate. This figure is a reproduction from Ref. [5].

Fig. 3 An example of transport analyses database created by TASK3D-a applications, (a) ion temperature, (b) electron temperature, (c) electron density, and then (d) ion heat diffusivity. These plots are reproduced from Ref. [9]. (M. Yokoyama)

Numerical Simulations on Plasma-wall Interaction

FDTD simulation on absorption of electromagnetic waves in tungsten fuzz structure

Tungsten fuzz structure was found in the plasma-wall interaction study in fusion science by the Takamura group at Nagoya University [1]. We, the PWI simulation group at NIFS, have been succeeding in creating the initial fuzz structure "in silico" by BCA-MD-KMC hybrid simulation [2]. The fuzz structure is regarded as a nuisance to confine the plasma in the nuclear fusion device, but as a by-product it has possibility to behave as a photonic crystal, because the optical absorptivity of the fuzz structure becomes almost 100% from visible to near infrared wavelength range. Thus it was known that the fuzz structurization increases the

aborptance of electromagnetic (EM) wave in tungsten. We revealed the mechanism of the high absorptivity of the tungsten fuzz structure by finite-difference time-domain (FDTD) simulation of simplified tungsten structures, i.e., the convex, the concave and the porous models [3]. Using FDTD simulation, we found that the nano-structures cause the enhancement of the EM-wave around them and then enhanced EM-wave generates the induced current in the surface of the tungsten. Thereby, the energy of the incident EM-field is transferred to the Joule heat derived by the induced current around the tungsten surface.

We, moreover, simulated "real fuzz structure" which was measured with transmission electron microscopy (TEM. Tecnai Spirit G2, 120 kV, \times 15 k, spot size 6) at the Yasunaga laboratory of Kyushu Institute of Technology. The three dimensional structure (Fig. 1) of the fuzz was reconstructed from tilt series (2 degrees from –64 to +64) by electron tomography (ECT using our developed Eos image processing package and eTomo provided by Dr. Mastronarde et al. at the University of Colorado). From the

simulation (Fig. 2), it is found that optical reflectance reduction is caused by confinement of the electromagnetic field in the tungsten fuzz structure as well as in the simplified tungsten structures.

Fig. 1 Tungsten fuzz structure by transmission electron microscopy (TEM. Tecnai Spirit G2, 120 kV, \times 15 k, spot size 6) at the Yasunaga laboratory of Kyushu Institute of Technology. The structure size is 202 nm \times 202 nm \times 530 nm.







Bulk

Fig. 2 Spatial-distribution of the time averaged electric field |E|. The regions surrounded by the closed pink curve indicates tungsten fuzz structures. The electric field is enhanced by the tungsten fuzz structure in the black region.

- [1] S. Takamura *et al.*, Plasma Fusion Res. **1**, 051 (2006).
- [2] A. M. Ito et al., Plasma and Fusion Res. 13, 3403061 (2018).
- [3] H. Nakamura *et al.*, International Conference on Plasma Surface Interactions in Controlled Fusion Devices (PSI-23), Princeton University, NJ, USA, 17–22 June 2018.

Neutron irradiation effects on bubble formed tungsten material

As a result of the nuclear fusion between deuterium and tritium, neutrons are generated with an energy of 14.1 MeV. By the neutron irradiation, nuclear transmutation and defects are induced in the divertor. These damages cause the change of property as plasma facing materials (ex., tungsten). Helium bubbles are generated in the surface of the tungsten, which is irradiated by helium plasma. We, therefore, investigate the neutron irradiation effects on bubble formed tungsten by Monte Carlo simulation code PHITS (Particle and Heavy Ion Transport code System)[4].

Tungsten is set in the region where z > 0. A circle with the radius of 5 cm is prepared as a neutron beam. The neutron emission points are set uniformly on the circular surface. Helium bubbles spread near the surface of the tungsten. The number and the positions of helium bubbles are determined by binary collision approximation based simulation [5]. From the simulation results (Fig. 3), we found that the helium bubbles affect trajectories of the neutrons and the electron generation at the surface of the helium bubbles [6].

- [4] T. Sato et al., J. Nucl. Sci. Technol. 55, 684 (2018).
- [5] S. Saito et al., Jpn. J. Appl. Phys. 55, 01AH07 (2016).





[6] S. Saito et al., 11th International Symposium on Advanced Plasma Science and its Applications for Nitrides and Nanomaterials, 12th International Conference on Plasma-Nano Technology and Science (ISPlasma2019/IC-PLANTS 2019), March 17-21, 2018 Nagoya Institute of Technology, Nagoya Japan.

(T. Sato, Yamagata University)

Molecular Dynamics Study on DNA Transformation by Tritium Disintegration

Towards better physical understanding of DNA transformation by tritium, we have examined double strand breaks of giant DNA molecules using a single molecule observation (SMO) technique at Toyama University [7]. However, separation of effects of ray irradiation (direct and indirect actions) from those of bond cleavage by tritium decay to inert helium-3 is difficult even if we use SMO method. Therefore, we have decided to adopt molecular dynamics (MD) simulation to elucidate the mechanism how beta-decays of substituted tritium give the effect to DNA [8].

We adopted a human telomeric DNA structure, where we replaced some hydrogen atoms in guanines to helium atoms. This replacement denotes the beta-decay of tritium into helium-3. The temperature of the system composed of DNA and water molecules is fixed to 310K with Langevin thermostat algorithm. Using NAnoscale Molecular Dynamics (NAMD) code[9]. Using these telomere structures where N hydrogen atoms are replaced with helium atoms in the guanine, we perform the MD simulation. To clarify the fragility of the DNA, we calculated the root mean square deviation (RMSD) for each N. In the case of N=0 (the original DNA), the DNA structure is saturated around 2 Å (Fig. 4). As N is increased, the RMSD becomes larger. From this result, we found that, as the number of the replaced helium increases, the double helix structure of the telomere becomes more fragile [10, 11].



- [7] Y. Hatano et al., Fusion Eng. Des. 146, 100 (2019).
- [8] S. Fujiwara et al., J. Adv. Simulat. Sci. Eng. 6(1), 94 (2019).
- [9] http://www.ks.uiuc.edu/Research/namd/

[10] H. Nakamura et al., 11th international Symposium on Advanced Plasma Science and its Applications for Nitrides and Nanomaterials, 12th International Conference on Plasma-Nano Technology and Science (ISPlasma2019/IC-PLANTS 2019), March 17-21, 2018 Nagoya Institute of Technology, Nagoya Japan.

[11] H. Nakamura et al., Jpn. J. Appl. Phys. (accepted), https://doi.org/10.7567/1347-4065/ab460d.

Fig. 4 The telomeric DNA structure. The length between DNA chains becomes larger as time passes. Wide gaps between chains are found clearly at the ends of DNA.