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Multiscale Modeling for Design of Fusion Materials
核融合材料設計に向けたマルチスケールモデリング

Kazunori Morishita[1], Yoshiyuki Watanabe[2] and Dai Hamaguchi[3]
森下和功，渡辺淑之，濱口　大

[1]*Institute of Advance Energy, Kyoto University, Gokasho, Uji, Kyoto 611-0011, Japan*
京都大学エネルギー理工学研究所　〒611-0011　京都府宇治市五ヶ庄

[2]*Research Reactor Institute, Kyoto University, 2, Asashiro-Nishi, Kumatori, Sennan, Osaka 590-0494 Japan*
京都大学原子炉実験所　〒590-0494　大阪府泉南郡熊取町朝代西2丁目

[3]*Japan Atomic Energy Agency, 2-166 Omotedate, Obuchi, Rokkasho, Aomori 039-3212, Japan*
原子力研究開発機構　〒039-3212　青森県上北郡六ヶ所村大字尾駮字表舘2番166

In order to realize a reliable fusion reactor, it is required to understand material behavior in fusion reactor environment accurately. In this report, an attempt is shown to predict material's response to fusion irradiation by theoretically-appropriate extrapolation of the irradiation data obtained at alternative facilities, in which a modeling approach from the multiscale viewpoint is important. A key to success of this study is a high performance computer installed at Rokkasho, Aomori in the BA-IFERC project.

1. The necessity of prediction of material behavior during irradiation

In a fusion reactor, the fist wall materials suffer from high energy neutron bombardment, which causes microstructural changes of the materials, resulting in degradation of the materials' performance. These can lead to serious problems in maintaining soundness of the fusion reactor. For a reliable fusion reactor, it is required to accurately predict material behavior in fusion reactor environment. In the present study, how to develop a methodology to predict material behavior in fusion reactor is introduced.

2. Multiscale feature of irradiation processes in material

In an irradiated material, many types of point defects such as vacancies, interstitials and helium gas atoms are produced by atomic displacement with incident high-energy neutrons at ps (pico second) and nm (nano meters), as shown in Figure 1. Those produced defects migrate by thermal diffusion at over sub μs (micro second) and sub μm and form defect clusters. These clusters cause microstructural change which is local disorder in atomic alignment of the material, leading to the materials' performance degradation at over ms and mm. As seen above, the irradiation processes in a material are temporally and spatially multi-scale phenomena [1]. Thus, understanding of the irradiation processes is attempted using a variety of experimental techniques and computational simulation techniques as shown in Figure 1, in which complementary use of those techniques is necessary. As part of that, a high performance computer introduced at the computational simulation centre (CSC) at Rokkasho in Aomori is brought into operation in the BA-IFERC project from next year.

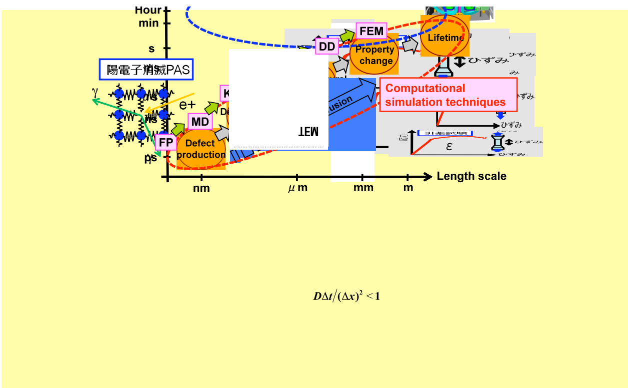

Fig.1 *Irradiation processes in material and multi-scale modeling approach*

3. The difference between alternative irradiation facilities and fusion reactor

As to experiments, much irradiation data has been obtained from alternative irradiation facilities such as existing material testing reactors and ion accelerators since there is no actual fusion reactor at present. However, those alternative facilities are absolutely different from an actual fusion reactor in irradiation conditions such as the damage rate (production rate of vacancies and interstitials) and helium gas production rate, as shown in Figure 2. Therefore, taking into account of the differences, theoretical extrapolation of the irradiation data obtained by the alternative facilities to irradiation data obtained by fusion reactor is required to predict the degradation of material's performance in fusion reactor.

The aim of the present study is to develop a modeling tool to interpret the irradiation data for the extrapolation, in which computational simulation approach with high performance computers based on the multi-scale viewpoint is necessary as described below.

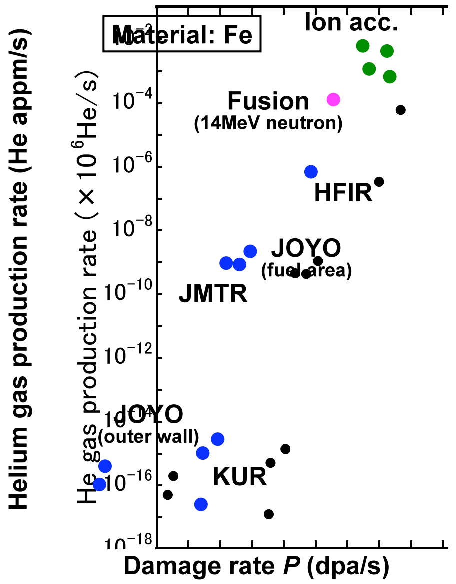

Fig.2 *Irradiation performance of irradiation facilities*

3. How to model the material behavior in fusion environment

The performance degradation of a material during irradiation results from the microstructural change associated with the defect cluster formation. Generally, the microstructural change can be described by rate theory based model on defect reactions [2]. As an example, a rate equation for vacancies can be simply given by:

$$\frac{dC_V}{dt} = P_V - D_V \nabla^2 C_V - \sum_j K_j C_V \qquad (1)$$

where the first term in right side P_V is estimated to the production rate of vacancies produced by the atomic displacement and corresponds to the damage rate as shown in Figure 2. Notice that this parameter reflects the performance of each irradiation facility. The second term is for defect migration in the material by thermal diffusion. And then, the third term is rate of defect cluster formation. It is here noted that the microstructural change of a material during irradiation is strongly associated with not only time but also P_V [3]. Keeping that in mind, the present study goes, for quantification of irradiation fields, through the following three steps:

(1) Evaluation of atomic displacement: The production rate of point defects by atomic displacement in fusion reactor is investigated by molecular dynamics method [4], in which great many atoms larger than 10 mega atoms should be treated because fusion neutron energy (14 MeV) is extremely much higher than fission neutron energy (2 MeV). From large-scale atomistic simulations, the point defect production rate is evaluated as a function of incident neutron energy and temperature.

(2) Evaluation of causal association of microstructural change with irradiation conditions: Formation of defect clusters such as interstitial loops, voids and helium bubbles is expected in irradiated materials for fusion application. In this step, response relation of the defect cluster formation to irradiation condition such as the point defect production rate, temperature and all should be theoretically investigated, in which large-scale kinetic Monte-Carlo analysis and rate theory analysis are mainly employed.

(3) Interpretation and realignment of the irradiation data: Based on the resultant information in step (2), existing irradiation date from the alternative irradiation facilities is theoretically interrelated and rearranged with the irradiation conditions. And then the extrapolation of the irradiation data to fusion environment is attempted.

Through the three above steps with help of the high performance computer introduced at CSC, it is attempted, for a reliable fusion reactor, to develop a methodology to predict material behavior in fusion reactor environment.

References

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