Derivation of condition for DPA conservation in kinetic Monte Carlo and transport Monte Carlo calculations for neutron irradiation damage estimation

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1. Introduction

The displacement per atom (DPA) plays a role as a unit of neutron irradiation damage in neutronic calculations. However, DPA itself does not contain any information about the target material in terms of mechanical property change. Recent progress in coarse grain methods enables to estimate the relationship between DPA and mechanical property change of the target material [1]. For example, the kinetic Monte Carlo (kMC) is one of the coarse grain methods which can be used for this purpose. The kMC can measure DPA regardless of neutronic calculation and provide a relationship between DPA and densities of defects induced by the collision between an impinging neutron and lattice atoms. The existing kMC codes used in irradiation damage calculation, such as BIGMAC or LAKIMOCA package [2], JERK [3] use a total neutron flux, which is calculated by a neutronic code to calculate DPA depending on the kind of irradiation that is simulated. However, the use of neutron flux as an input parameter of kMC does not satisfy the condition for consistency of DPA calculation between neutronics and kMC. In this paper, a condition for satisfying the consistency in terms of DPA between transport MC (tMC) and kMC is derived.

2. Displacement and DPA

According to the NRT formula, the number of displacements by recoil atom having kinetic energy T is given by

$$\nu_R(T) = \frac{0.8T}{2.0E_d} \tag{1}$$

where E_d is the threshold energy for displacement.

In tMC, the neutron flux $\phi(E)$ has the meaning of the average number of neutrons that penetrates a sphere of unit cross section in common, cm^2 , per one source neutron. Therefore, total number of displacements between T and T+dT which can be obtained from tMC is given by

$$\nu_R(T)dT = N\sum_i \frac{0.8T}{2.0E_d}\int_0^\infty \phi(E)\sigma_i(E)f_i(E\to T)dEdT \tag{2}$$

where i is the collision type index, σ_i is the microscopic cross section for collision type i, f_i is transfer kernel for collision type i and N is the number density of the target material. Then, DPA per a source neutron can be calculated by

$$\bar{d}_{tMC} = \sum_i \int_0^\infty \frac{0.8T}{2.0E_d}\int_0^\infty \phi(E)\sigma_i(E)f_i(E\to T)dEdT \tag{3}$$

3. DPA calculation in transport Monte Carlo

Eq. (3) can be rewritten as follows:

$$\bar{d}_{tMC} = \int_0^\infty \nu_R(T)R(T)dT \tag{4}$$

where $$R(T) = \sum_i \int_0^\infty \phi(E)\sigma_i(E)f_i(E\to T)dE$$

which is called recoil atom spectra.

Now let's suppose that the incident rate of neutron is I per second. Then, DPA per a second is

$$\bar{d}_{tMC} = I\times\int_0^\infty \nu_R(T)R(T)dT \tag{5}$$

4. Dpa calculation in kinetic Monte Carlo

Originally, DPA is a function of time t and recoil energy T. Therefore, in kMC, DPA can be defined by

$$d_{kMC}(T,t) = \frac{\nu_{kMC}(T,t)}{N_{sys}} \tag{6}$$

where N_{sys} is the number of atoms in the simulation box that is simulated now.

Let's suppose that the probability density function for $\nu_{kMC}(T,t)$ is given by $p(T,t)$. Then the average value of DPA for all recoil energies and time is given by

$$\bar{d}_{kMC} = \int_0^\infty\int_0^\infty d_{kMC}(T,t)p(T,t)dTdt \tag{7}$$

In the frame of kMC for irradiation damage calculation, it's assumed that the all events causing any transition of state of the system are infrequent. This means that it's very hard to take place simultaneously for any events in this system. Under this assumption, the time and recoil energy can be treated separately for both $\nu_{kMC}(T,t)$ and $p(T,t)$.

$$p(T,t) = p_R(T)\,p_t(t) \tag{8}$$

$$d_{kMC}(T,t) = \frac{\nu_{kMC}(T,t)}{N_{sys}} = \frac{\nu_R(T)\nu_t(t)}{N_{sys}} \tag{9}$$

From the Eq. (7), Eq. (8) and Eq. (9),

$$\bar{d}_{kMC} = \int_0^\infty \frac{\nu_R(T)}{N_{sys}} p_R(T)dT \int_0^\infty \nu_t(t)p_t(t)dt \tag{10}$$

Eq. (10) contains the actual algorithm of kMC. In a kMC simulation, the recoil energy T is chosen from a recoil atom spectrum. And the corresponding elapsed time Δt for that event is sampled out independent of recoil energy T. This means that the kMC simulations can be regarded as integration of Eq. (10). Therefore, $p_R(T)$ is given by

$$p_R(T) = \frac{R(T)}{R} \tag{11}$$

where $R \equiv \int_0^\infty R(T)dT$ which is called the total recoil atom density. This can be also regarded as a collision density between neutron and the target atoms. From Eq. (10) and Eq. (11),

$$\bar{d}_{kMC} = \frac{1}{N_{sys}R} \int_0^\infty \nu_R(T)R(T)dT \int_0^\infty \nu_t(t)p_t(t)dt \tag{12}$$

5. Condition for conserving DPA in tMC and kMC calculations

For consistency between tMC and kMC in terms of conservation of DPA, $\bar{d}_{tMC}$ must be equal to $\bar{d}_{kMC}$. Therefore, from Eq. (5) and Eq. (12),

$$\int_0^\infty \nu_t(t)p_t(t)dt = RN_{sys}I \tag{13}$$

If $\nu_t(t)$ is assumed constant for all simulation time, then,

$$\nu_t = RN_{sys}I \tag{14}$$

Therefore, the production rate must be determined by Eq. (14) to preserve DPA in both tMC and kMC.

6. Test of Consistency

To verify whether DPAs calculated by the traditional method and the proposed method are the same, the formula introduced above are applied to a test problem which is to examine DPA evolution as a function of time in a structural material of a Helium Cooled Molten Lithium Test Blanket Module (HCML TBM) for ITER. In the neutronic calculation, the neutron spectrum was obtained by the Monte Carlo code. The recoil atom spectrum and time averaged DPA per source neutron was directly calculated by Eq. (3) using the ENDF-B/VII data and the NJOY code. A OKMC simulation was performed at 373K for a pure $200a_0 \times 200a_0 \times 200a_0$ Fe box where a_0 is a lattice parameter of Fe. The number of incident neutrons is assumed arbitrarily to be 10^{25} per sec. Eq. (11) was used as a PDF for sampling of the recoil energy. Eq. (14) is transformed into a production rate of defects cascades. Fig. 1 shows each path of DPA evolution of 10 OKMC simulations. Because kMC is inherently stochastic, all paths are different whenever it's performed.

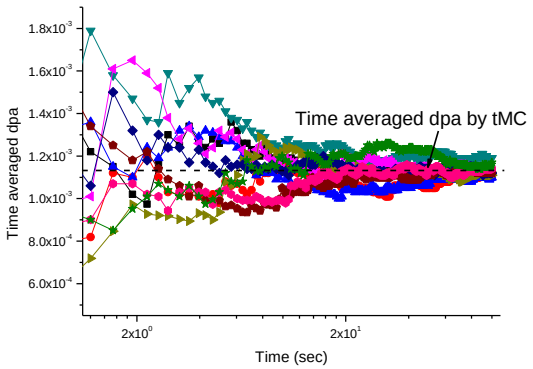

Fig 1. DPA evolution as a function of time for 10 OKMC simulations and time averaged dpa by tMC

It is, however, clearly seen that time averaged DPAs always converge to the one calculated by the neutronic code. This means that the introduction of Eqs. (11) and (14) ensures that the DPA evolution in OKMC always satisfies the consistency with the neutronic calculation.

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