JOURNAL OF NANO- AND ELECTRONIC PHYSICS
Vol. **11** No 4, 04025(4pp) (2019)

ЖУРНАЛ НАНО- ТА ЕЛЕКТРОННОЇ ФІЗИКИ
Том **11** № 4, 04025(4cc) (2019)

Effect of the Temperature Change of Material Test Reactor on Calibration of Cluster Dynamics for Neutron Irradiation Pure Iron

O.R. Gokhman, M.S. Kondria

South Ukrainian National Pedagogical University, 26, Staroportofrankivska St., 65020 Odesa, Ukraine

(Received 03 June 2019; revised manuscript received 07 August 2019; published online 22 August 2019)

Cluster dynamics (CD) simulation is used to study the effect of the temperature T change of reactor pressure vessel (RPV) on the evolution of vacancy clusters (VC) and self-interstitial atom clusters (SIAC) in neutron irradiation pure iron in material test reactor (MTR) BR-2 (Mol, Belgium). During operation time of BR-2, T increases from 300 K to 573 K in the first 19 hours, does not change in the next 370 hours and decreases then to 373 K in the last 7 hours. The time evolution of concentrations of single vacancies, C_{1v}, single self-interstitial atoms, C_{1i}, of VC, C_{nv}, and SIAC, C_{ni}, in pure iron under neutron irradiation in the MTR BR-2 for neutron flux of 1.39×10^{-7} dpa/s in the range fluence from 0.026 to 0.19 dpa are determined by CD simulation for approach on the constant T as well as with taking into account T change of RPV. Then the dose dependences of number density and mean size of SIAC are calculated. The new calibration of defect structure model has been performed from the comparison of experimental transmission electron microscopy (TEM) data and CD simulation results. It was found the migration energy of a vacancy in iron which provides the best coincidence of experimental data and CD results. The difference between predictions of CD model on dose dependences of the number density and mean size with the constant temperature and model with taking into account the change temperature at the beginning and at the end of operation time of MTR BR-2 has been analyzed.

Keywords: Cluster dynamics, Pure iron, Change of temperature, Vacancy clusters, Self-interstitial clusters.

DOI: 10.21272/jnep.11(4).04025 PACS numbers: 61.80.Hg, 61.80.Az, 61.72.Ji, 61.82.Bg

1. INTRODUCTION

In the last several decades, the actual issue of reactor material science is to monitor mechanical properties and to increase the life-time of the reactor pressure vessel (RPV) to 60-80 years. There are several approaches. They are investigation of the RPV after it's decommissioning [1, 2]; use of the ion model irradiation [3, 4]; study of the surveillance samples that are installed in the set of places of the material test reactors (MTR) [5-8]. The effect of difference in fluxes for the commercial nuclear reactor and MTR on the reliability of the long-term behavior forecast of commercial reactor is discussed in [9-12]. The cluster dynamics (CD) model has been used to simulate the evolution of point defect clusters in irradiated pure iron [13-15]. The experimental data for commercial pure iron ($C < 30$ ppm) neutron irradiated in MTR BR-2 (Mol, Belgium) with fluence in the range from 0.026 to 0.2 dpa and flux of 1.39×10^{-7} dpa/s are used to calibrate the CD model [15]. The assumption on the constant temperature ($T = 573$ K) of RPV is used in [15]. However, in fact T increases from 300 K to 573 K during about 19 hours, does not change up to time of 370 hours and then decreases to about 373 K during about 7 hours in MTR BR-2 (Fig. 1). The aim of our present study is to clarify the calibration of CD model [15] by taking into account the discussed change of temperature.

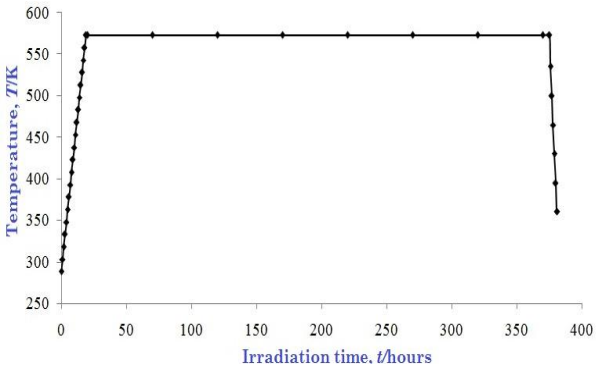

Fig. 1 – The change of temperature of reactor pressure vessel of MTR BR-2 during irradiation

2. CD SIMULATION AND DISCUSSION

CD master equation is valid for the case of non-spatially correlated and low concentrated cluster systems. Usually, these assumptions are realized for point defect clusters in irradiated materials [16, 17]. In our study, CD master equation for pure iron has been taken from [15] as a system of ordinary differential equations related to the concentration of single vacancies, C_{1v}, single self-interstitial atoms, C_{1i}, vacancy clusters (VC) with n vacancies, C_{nv}, and self-interstitial clusters (SIAC) with n self-interstitial atoms, C_{ni}:

$$\frac{dC_{1v(i)}}{dt} = \eta G_{dpa}\left(1 - f_{vcl(icl)}\right) - \frac{4\pi r_{rec}\left(D_v + D_i\right)C_{1v}C_{1i}}{\Omega_{Fe}} - \rho_d Z_{v(i)}\left(1 + \frac{6\left(\rho_d Z_{v(i)}\right)^{-0.5}}{d}\right)D_{v(i)}\left(C_{1v(i)} - C^e_{1v(i)}\right)$$
$$- 4\beta^{v(i)}_{1v(i)}C_{1v(i)} + 4\alpha^{v(i)}_{2v(i)}C_{2v(i)} - \sum_{n=2}\beta^{v(i)}_{nv(i)}C_{nv(i)} + \sum_{n=3}\alpha^{v(i)}_{nv(i)}C_{nv(i)} + \beta^{i(i)}_{2v(i)}C_{2v(i)} - \sum_{n=2}\beta^{v(i)}_{ni(i)}C_{ni(i)} \quad (1)$$

$$\frac{dC_{2v(i)}}{dt} = G_{2v(i)} + 2\beta^{v(i)}_{1v(i)}C_{1v(i)} - 2\alpha^{v(i)}_{2v(i)}C_{2v(i)} - \beta^{v(i)}_{2v(i)}C_{2v(i)} + \alpha^{v(i)}_{3v(i)}C_{3v(i)} - \beta^{i(i)}_{2v(i)}C_{2v(i)} + \beta^{i(i)}_{3v(i)}C_{3v(i)}\,, \tag{2}$$

$$\frac{dC_{nv(i)}}{dt} = G_{nV(I)} + \beta^{v(i)}_{(n-1)v(i)}C_{(n-1)v(i)} + \left(\beta^{i(v)}_{(n+1)v(i)} + \alpha^{v(i)}_{(n+1)v(i)}\right)C_{(n+1)v(i)} - \left(\beta^{v(i)}_{nv(i)} + \beta^{i(i)}_{nv(i)} + \alpha^{v(i)}_{nv(i)}\right)C_{nv(i)} \text{ for } n > 2\,. \tag{3}$$

Here η is efficiency coefficient: $\eta = 0.3$, f_{vcl} (f_{icl}) is the fraction of vacancies (SIAs) formed by clusters at the cascade stage: $f_{vcl} = 0.07$ and $f_{icl} = 0.2$; $G_{nv(i)}$ is the production rate of VC(SIAC) with size n at the cascade stage: $G_{2v} = G_{6v}\eta f_{vcl}G_{dpa}/8$ $G_{nv} = 0$ ($n \neq 2.6$); $G_{2i} = G_{4i} = \eta f_{vcl}G_{dpa}/6$, $G_{ni} = 0$ ($n \neq 2.4$); Ω_{Fe} is the atomic volume of bcc iron, ρ_d is the dislocation density, d is the mean grain size, r_{rec} is the recombination radius for Frenkel' pair, $C^e_{1v(i)}$ is the thermal equilibrium concentration of vacancies (SIA), Z_v and Z_i are the capture efficiency of vacancy and SIA, respectively, by dislocation net, $D_{v(i)}$ is the diffusion coefficient of the vacancy (SIA) calculated according to the Eq. (4):

$$D_{v(i)} = D_{v(i)0}\exp\left(-\frac{E_{mv(i)}}{k_BT}\right), \tag{4}$$

$D_{v(i)0}$ is the pre-factor, k_B is the Boltzmann constant, $E_{mv(i)}$ is the migration energy of vacancy (SIA); $\beta^{v(i)}_{ni}$ are the attachment coefficients of the point defects by the planar SIAC calculated from the Eq. (5); attachment coefficients of the point defects by the spherical VC are calculated from the Eq. (7).

$$\beta^{v(i)}_{ni} = (2\pi r_{ni}D_{v(i)}C_{1v(i)}/\Omega_{Fe})\cdot Z^{v(i)}_{n}\,, \tag{5}$$

where $Z^{v(i)}_{ni}$ is the capture efficiency of vacancy (SIA) by SIAC calculated from the Eq. (6):

$$Z^{v(i)}_{ni} = Z_{v(i)} + \left[\left(\frac{b}{8\pi a}\right)^{0.5}\cdot z_{fv(i)} - Z_{v(i)}\right]/n^{0.35}\,. \tag{6}$$

Here a is the lattice parameter of bcc pure iron, b is the Burgers vector and $z_{fv(i)} = 35$ (42) for vacancy (SIA).

$$\beta^{v(i)}_{nv} = (4\pi R_{nv}D_{v(i)}C_{1v(i)}/\Omega_{Fe})\,, \tag{7}$$

$\alpha^{v(i)}_{ni(i)}$ are the emission coefficients of vacancy (SIA) from the VC (SIAC) calculated in accordance with the detailed balance principle via $\Delta G_v(n)$, in the case of VC and via the E_{bni}, in the case of SIAC:

$$\alpha^{v}_{nv} = \beta^{v}_{(n-1)v}\cdot\exp\frac{\Delta G_v(n) - \Delta G_v(n-1)}{k_BT}\,, \tag{8}$$

$$\alpha^{i}_{ni} = \frac{\beta^{i}_{(n-1)i}}{C_{1i}}\cdot\exp\left(-\frac{E_{bni}}{k_BT}\right). \tag{9}$$

Here

$$\Delta G_v(n) = -n\Delta\mu_v + 4\pi R^2_{nv}\gamma\,, \tag{10}$$

where $\Delta G_v(n)$ is the difference in the free energy of the spherical VC of size n and the system of n free vacancies; $\Delta\mu_v$ is the difference in the chemical potential of the vacancy in the VC and in the ambient space; R_{nv} is the radius of VC of size n, γ is the specific energy of VC in iron. E_{bni} is calculated from the Eq. (11):

$$E_{bni} = E_{fi} + \frac{E_{b2i} - E_{fi}}{2^{\frac{2}{3}} - 1}\left[n^{\frac{2}{3}} - (n-1)^{\frac{2}{3}}\right]. \tag{11}$$

It was found that decrease of E_{vm} from 1.3 eV (Table 1) to 0.62 eV provides the best fit of CD results for model with the change of temperature (Fig. 1) to the experimental transmission electron microscopy (TEM) data [17] on mean size and number density of SIAC: 5 nm and 0.95×10^{21} m^{-3}, 7 nm and 1.30×10^{21} m^{-3}, and 10 nm and 4.0×10^{21} m^{-3} for 0.051, 0.10 and 0.19 dpa, respectively. The found value of E_{vm} of 0.62 eV in the present CD simulations corresponds better to the purity of iron in [12, 17] ($C < 30$ ppm) than the value of 1.3 eV found in previous CD simulation [15].

The dose dependences of mean size, D_{SIAC}, and number density, N_{SIAC}, calculated by CD simulations as well as the TEM data [17] are presented in Fig. 2 and Fig. 3. CD simulations for model with assumption of the constant temperature of RPV of MTR BR-2 result in underestimation of D_{SIAC} and N_{SIAC} values in comparison with both TEM data and CD simulations with temperature change according to Fig. 1.

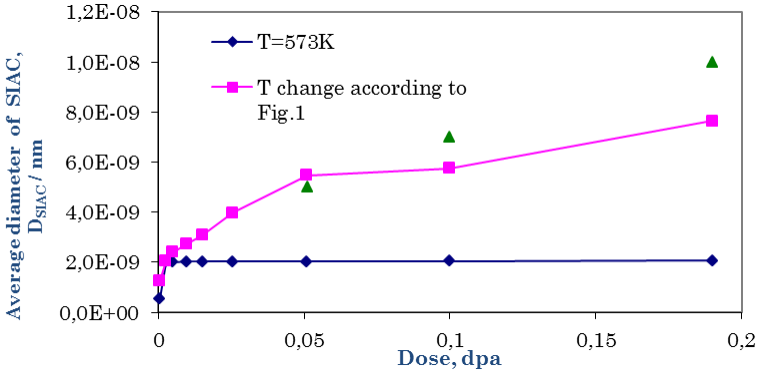

Fig. 2 – Dose dependence of mean size of SIAC, D_{SIAC}, calculated according to the assumption of the constant temperature and with taking into account the temperature change according to Fig. 1 in comparison with TEM data

Table 1 – Material parameters of pure iron in CD model [15]

Parameter	Value	References
Vacancy formation energy, E_{fv}	1.60 eV	[8, 9]
Binding energy of vacancy dimmer, E_{b2v}	0.608 eV	[9]
Vacancy migration energy, E_{mv}	1.30 eV	[8, 9]
Vacancy pre-exponential, D_{vo}	2.0×10^{-8} m²/s	[8, 9]
Interstitial formation energy, E_{fi}	3.05 eV	[9]
Binding energy of interstitial dimmer, E_{b2i}	0.8 eV	[8, 9]
Interstitial migration energy, E_{mi}	0.30 eV	[8, 9]
Interstitial pre-exponential, D_{io}	4.0×10^{-8} m²/s	[8, 9]
Recombination radius, r_{rec}	0.65 nm	[8, 9]
Capture efficiency for vacancy by dislocation net, z_v	1.0	[8, 9]
Capture efficiency for interstitial by dislocation net, z_i	1.2	[8, 9]
Burgers vector of the loop assumed to be prismatic, b	0.2 nm	[8, 9]
Dislocation density, ρ_d	0.7×10^{14} m^{-2}	[9]
Average grain size, d	2.5×10^{-4} m	[9]
Lattice parameter of iron, a	0.2866 nm	[8, 9]

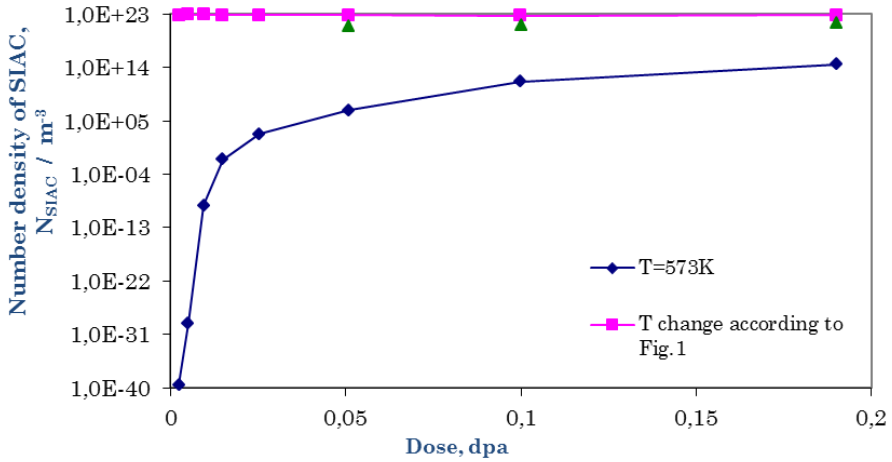

Fig. 3 – Dose dependence of number density of SIAC, N_{SIAC}, calculated according to the assumption of the constant temperature and with taking into account the temperature change according to Fig. 1 in comparison with TEM data

3. CONCLUSIONS

It is proved that the study of the temperature change at the beginning and at the end of exploitation on the defect structure of reactor pressure vessel (RPV) of material test reactor (MTR) BR-2 is the actual issue of material science. In particular, it was found that the cluster dynamics (CD) simulation for the model, which takes into account the above-mentioned change of temperature, results in the best fit of CD results to the experimental transmission electron microscopy (TEM) data if the migration energy of vacancy, E_{mv}, is about 0.62 eV. The latter value corresponds better to the purity of investigated iron ($C < 30$ ppm) than E_{mv} of about 1.3 eV, which provides the best fit of CD results to the experimental TEM data for the model, which takes the assumption on the constant temperature of RPV of MTR BR-2.

REFERENCES

1. A. Ulbricht, E. Altstadt, F. Bergner, H. Viehrig, U. Keyderling, *J. Nucl. Mater.* **416**, 111 (2011).
2. M. Jenkins, Z. Yao, M. Hernandez-Maoyoral, M. Kirk, *J. Nucl. Mater.* **389**, 197 (2009).
3. G. Was, M. Hash, R. Odette, *Phil. Mag.* **85**, 703 (2006).
4. C. Heintze, F. Bergner, S. Akhmadaliev, *J. Nucl. Mater.* **472**, 196 (2016).
5. A. Hrytsenko, V. Demekhyn, V. Yl'kovych, V. Bukanov, E. Vasyl'eva, *Yaderna ta radiatsiyna bezpeka* **50**, 29 (2011) [In Ukrainian].
6. V. Dem'okhin, V. Il'kovych, V. Bukanov, *Yaderna ta radiatsiyna bezpeka* **54**, 21 (2012) [In Ukrainian].
7. S. Jumel, J.V. Duysen, *J. Nucl. Mater.* **366**, 256 (2007).
8. V. Slugen, O. Gokhman, S. Pecko, S. Soyak, F. Bergner, *Radiat. Eff. Defect. S.* **171**, 231 (2016).
9. G. Odette, T. Yamamoto, D. Klingensmith, *Phil. Mag.* **85**, 779 (2005).
10. S. Shu, N. Almirall, P. Wells, T. Yamamoto, G. Odette, D. Morgan, *Acta Materialia* **157**, 72 (2018).
11. A. Wagner, F. Bergner, R. Chaouadi, H. Hein, M. Hernandez-Mayoural, M. Serrano, A. Ulbricht, E. Altstadt, *Acta Materialia* **104**, 131 (2016).
12. M. Kondria, A. Gokhman, *Radiat. Eff. Defect. S.* **174**, 56 (2019).
13. A. Hardouin Duparc, C. Moingeon, N. Smetanynski-de Grande, A. Barbu, *J. Nucl. Mater.* **302**, 143 (2002).
14. E. Meslin, A. Barbu, L. Boulanger, B. Radiguet, P. Pareige, K. Arakawa, C. Fu, *J. Nucl. Mater.* **382**, 190 (2008).
15. A. Gokhman, F. Bergner, *Radiat. Eff. Defect. S.* **165**, 216 (2010).
16. A. Gokhman, J. Boehmert, *Radiat. Eff. Defect. S.* **158**, 499 (2003).
17. M. Lambrecht, M. Jardin, A. Almazouzi, *phys. status solidi* **4**, 3477 (2007).

Вплив зміни температури науково-дослідного реактора на калібрування кластерної динаміки чистого заліза, яке опромінено нейтронами

О.Р. Гохман, М.С. Кондря

Південноукраїнський національний педагогічний університет ім. К.Д. Ушинского, вул. Старопортофранківська 26, 65020 Одеса, Україна

Моделювання кластерної динаміки (КД) використовується для вивчення впливу зміни температури T корпусу реактора на еволюцію кластерів вакансій (ВК) та кластерів міжвузельних атомів (КМА) в чистому залізі при нейтронному опроміненні у науково-дослідному реакторі BR-2 (Мол, Бельгія). Під час роботи реактору BR-2 T збільшується від 300 K до 573 K в перші 19 годин, не змінюється у наступні 370 годин і зменшується до 373 K за останні 7 годин експлуатації. Часова еволюція концентрацій поодиноких вакансій, C_{1v}, поодиноких міжвузельних атомів, C_{1i}, ВК, C_{nv} та КМА, C_{ni}, у чистому залізі при опроміненні нейтронами у науково-дослідному реакторі BR-2 для потоку нейтронів 1.39×10^{-7} dpa/s у діапазоні флюенсів від 0.026 до 0.19 dpa визначаються шляхом моделювання КД для підходу щодо незмінної T, а також з урахуванням зміни T корпусу реактора. Потім розраховується дозова залежність чисельної щільності та середнього розміру КМА. Виконано нове калібрування моделі дефектної структури з порівнянням даних експериментальної просвічуючої електронної мікроскопії та результатів моделювання методом КД. Встановлено енергію міграції вакансії в залізі, яка забезпечує найкраще збіг експериментальних даних і результатів КД. Проаналізовано різницю між прогнозами КД щодо дозової залежності щільності чисел і середнього розміру КМА для моделі з постійною температурою та моделі з урахуванням зміни температури на початку і в кінці експлуатації науково-дослідного реактора БР-2.

Ключові слова: Кластерна динаміка, Чисте залізо, Зміна температури, Кластери вакансій, Кластери міжвузельних атомів.