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Multiscale modeling study of pulsed damage accumulation in α-Fe under inertial fusion conditions

J.M. Perlado [a], D. Lodi [a,b,*], E. Domínguez [a], J. Prieto [a], M.J. Caturla [c], Tomas Díaz de la Rubia [c]

[a] *Instituto de Fusión Nuclear, Universidad Politécnica de Madrid, c/Jose Gutierrez Abascal 2, 28006 Madrid, Spain*
[b] *SCK-CEN, Boeretang 200, 2400 Mol, Belgium*
[c] *Lawrence Livermore National Laboratory, Livermore, CA 94550, USA*

Abstract

Reduced activation ferritic–martensitic (RAFM) steels are being considered as candidate materials for the first structural wall of a future fusion reactor, due to their high resistance to neutron irradiation. A combination of molecular dynamics and kinetic Monte Carlo has been utilized to analyze and assess the change and evolution of the microstructure in irradiated α-Fe, the main component of RAFM steels. We discuss how the pulse frequency, 1 and 10 Hz, may affect the damage production and accumulation. Dose rates of 0.1 and 0.01 dpa/s will be considered in order to represent the damage suffered by a protected first structural wall. These results will be compared with previous work on the subject and with those achieved with continuous irradiation at similar average dose rate.

1. Introduction

Radiation is well known to induce an alteration of the materials microstructure whose long-term evolution leads to the modification of the macroscopic features. Multiscale modeling is demonstrating a large potential for studying those effects [1–4]. Many studies have been conducted to analyze the effect on materials of continuous irradiation with energetic particles (neutrons, others) and according to different temporal distributions. Many uncertainties still exist when a fusion reactor (e.g. inertial) environment study is considered. The high neutron energy peak, 5 MeV for a protected and 14 MeV for an unprotected wall, and the pulsed nature of irradiation are the principal factors that need to be studied in order to evaluate the response of the first structural wall of a future inertial fusion energy (IFE) reactor.

The fundamental requirements for a first wall material are [5] resistance to 14 MeV neutron induced displacement damage and mechanical and physical properties adequate to meet conditions imposed by the 30 dpa dose expected during reactor lifetime.

In this paper we analyze the effect of pulsed irradiation on α-Fe, the main component of steels which are considered in some designs of future inertial fusion reactors [6]. We will consider the effect of two dose rates and two different frequencies on defect cluster accumulation, with the intention of reproducing the damage suffered by a first structural wall that will be exposed to high-energy 14 MeV neutrons irradiation.

The characteristics of the radiation environment simulated here are extensively described in a previous paper [7] and will not be reported here.

2. Simulation model

The multiscale modeling approach makes use of a set of linked programs to bridge the wide range of time and spatial scales that radiation damage involves.

* Corresponding author. Address: Instituto de Fusión Nuclear, Universidad Politécnica de Madrid, c/Jose Gutierrez Abascal 2, 28006 Madrid, Spain. Fax: +34-91 336 3002.
E-mail address: dario@denim.upm.es (D. Lodi).

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The spatial and energetic distribution of the subcascade generated by a primary knock-on atom (PKA) is calculated with the program TRIM [8], Fig. 1. Along with a cascade data base partly calculated by the molecular dynamics (MD) code MDCASK [9] and partly from the literature [10], this forms the input for the program that builds the pulse.

The number of PKAs forming the pulse is a function of the selected dose rate per pulse, the pulse deposition time, and the kinetic Monte Carlo (KMC) simulation box.

The result of this first step in the damage simulation is a number of point and clustered defects that are inserted into the KMC box at the required rate.

In the KMC simulation box we follow the evolution of the microstructure with the program BIGMAC [11], an efficient KMC code that generates the behavior and lifetime of the chosen defect population through a well-defined sequence of events, based on a known probability distribution. MC is, because of this characteristic, a suitable and very useful tool to study the evolution of the microstructure of an irradiated material extended to long times. In order to be able to perform our KMC simulations, a well-defined series of input data is needed. The various species that constitute the defect population, the characteristic energies of each species and the reactions that may occur between each one of them are required. In our simulation we have considered single point defects (vacancy and interstitial) and point defects clusters, taking each size as a different object, and substitutional impurities as well. Impurities have been considered immobile, transparent to vacancies and capable of reacting only with interstitials with a binding energy of 1.0 eV. Seven possible events have been allowed on: (1) diffusion, (2) clustering of defects of the same type, (3) dissociation of a single defect from a cluster, (4) annihilation of defects of opposite type, (5) annihilation of defects at a sink (grain boundary), (6) trapping of an interstitial by an impurity, (7) new cascade formation.

Each object in the simulation box has an associated set of probabilities corresponding to the undergoing events. All the interstitial clusters have been considered mobile in three dimensions for sizes up to four, and one dimension for bigger clusters; whereas only vacancy clusters up to sizes of three are allowed to undergo three dimensional migration.

All simulations have been conducted in a 300 nm cubical box, with periodic boundary conditions applied in the three directions. Dose rates per pulse of 0.1–0.01 dpa/s were considered, corresponding to those computed in protected walls [12], along with pulse frequencies of 1–10 Hz and temperatures of 300 and 600 K.

The high energy of the PKA, 150 keV, and its numerous associated defects introduced in the box per pulse, together with the low interstitial migration energy, slowed the simulation down and made computational time long. For this reason the only results obtained at 300 K are currently available.

3. Results

The results, which will be represented in terms of clusters size and concentration, have been obtained after 1000 pulses in the 'high' pulse dose rate and of 10 000 in the 'low' pulse dose rate case, each of which gives a total dose of 1×10^{-4} dpa. The pulse deposition time in each case was 1 μs, which makes the dose accumulated in the pulse 10^{-7} and 10^{-8} dpa, respectively.

A key point for analyzing and understanding the obtained results is the relation between the external magnitudes – pulse frequency and deposition time – and the magnitudes characteristic of the modeling of the

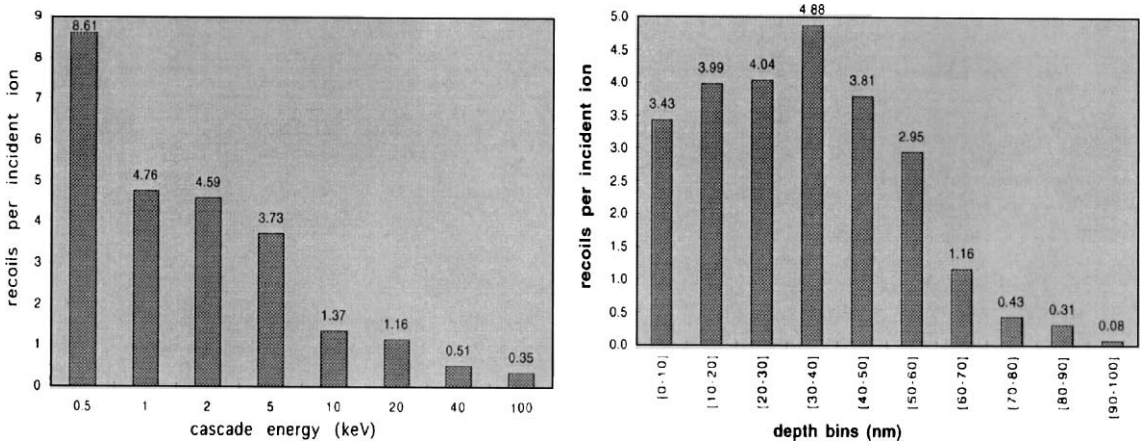

Fig. 1. Spatial and energy distributions of recoils generated by 150 keV Fe^{+} in Fe.

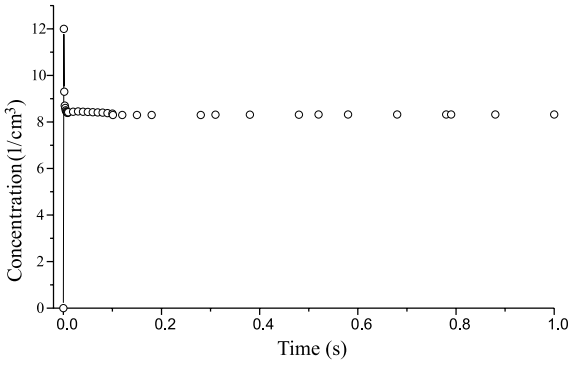

Fig. 2. Vacancy cluster concentration vs. time at 1 Hz.

material – such as defect diffusion and recombination time.

Interstitials rapidly migrate to sinks and then the recombination phase with the vacancies begins. For vacancies it is the opposite; the first process is recombination and then the less probable and very slow migration takes place.

Fig. 2 shows the evolution of vacancy cluster concentration during one pulse. There is, a very fast interstitial–vacancy recombination process that leads to a steep decrease in the concentration. After all the interstitials have disappeared in sinks, have interacted with impurities or have reacted with vacancies, the vacancy concentration tends to remain stable. The most probable events that can occur in this situation are di-vacancy migration, and di-vacancy splitting into two single-vacancies. The results of the first event would be a decrease in vacancy cluster concentration due to the fact that it is highly probable that during migration the di-vacancy cluster could interact with another vacancy and form a three-vacancy cluster whose probability of splitting or diffusing is much lower. The second mechanism would lead to an increase of vacancy cluster concentration. In this case the single-vacancy is not very likely to move at the temperature considered in the simulation; but again we have to consider the fact that vacancies are situated in a very small region and so the probability is not negligible for a single-vacancy, resulting from the splitting of a di-vacancy, to find another vacancy in the capture volume. In our simulations we have noted that the vacancy cluster concentration remains basically stable and in some cases shows a little decrease during a single pulse. The first result can be ascribable to the mechanism explained before, splitting and recombination, or simply to an immobility of the vacancies. The decrease in vacancy cluster concentration must in turn be attributed to a di-vacancy migration and final recombination with another vacancy to form a bigger cluster.

Interstitial lifetime is so short [13] that pulse frequency plays no role in the accumulation. For this reason no differences appear in the trapped interstitial concentration. When plotting vacancy cluster accumulation versus dose (Fig. 3) no significant difference was observed between different dose rates per pulse and pulse frequencies at the accumulated dose in these simulations. The observable differences can be attributed to a repetition rate effect, which can be summarized by saying that the more time that elapses between pulses, the more probable it is for a di-vacancy (that has the lowest migration energy) to undergo migration. What is more likely to happen when the di-vacancy migrates is a

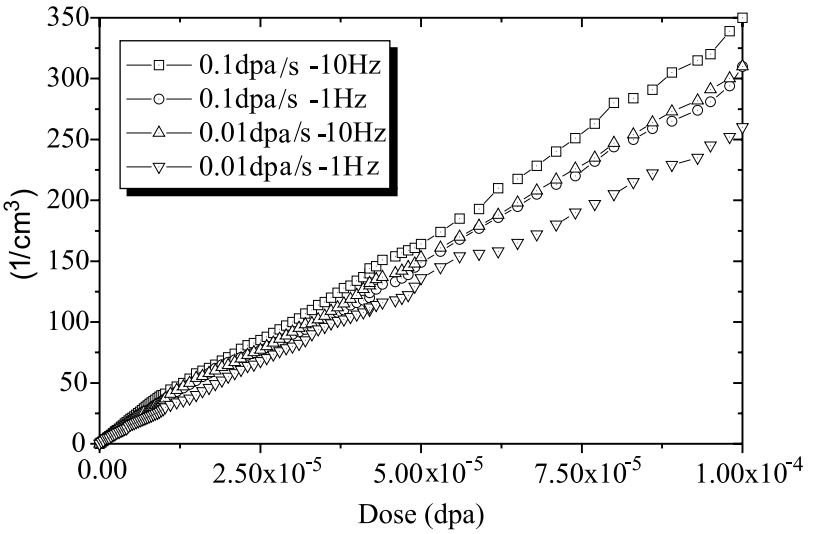

Fig. 3. Vacancy cluster concentration vs. dose.

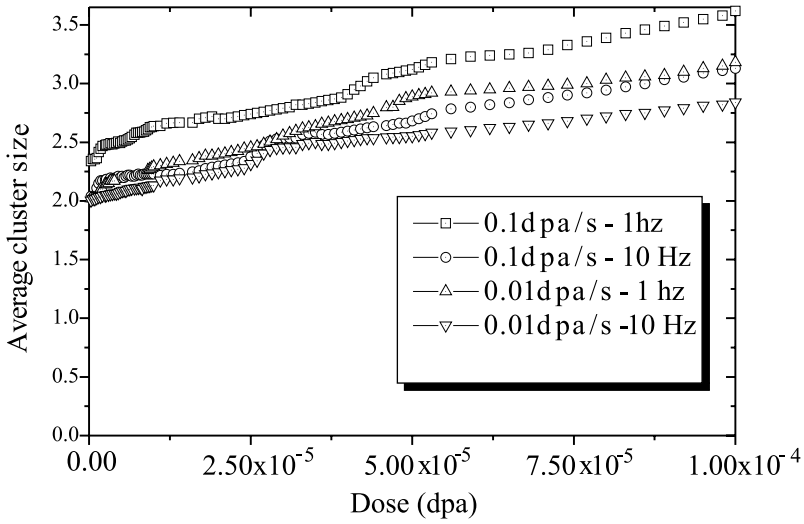

Fig. 4. Average vacancy clusters size vs. dose.

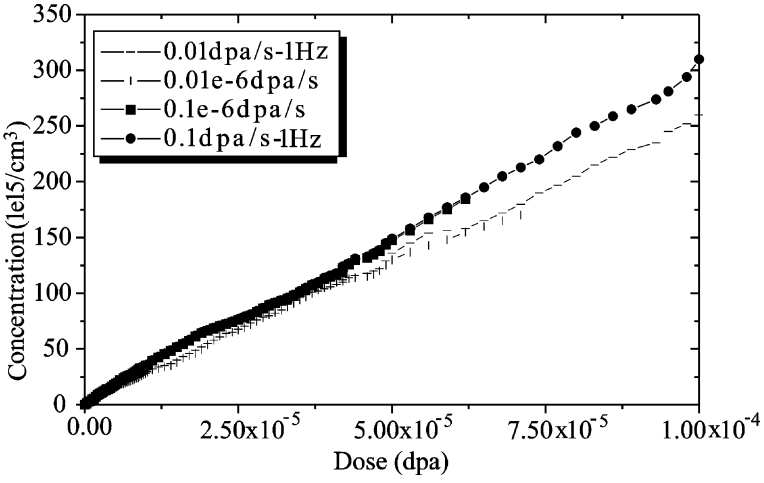

Fig. 5. Comparison between pulsed and continuous irradiation (0.1×10^{-6}–0.01×10^{-6} dpa/s).

reaction with a vacancy to form a bigger cluster, raising the average cluster size (Fig. 4) and diminishing the vacancy cluster concentration. The spatial distribution of the defects introduced in the KMC box reflects the characteristics of the collisional cascade in iron with vacancies in the core region and an interstitial shell [14].

Fig. 5 shows the comparison between pulsed and continuous irradiation. We have compared the effect of pulsed irradiation with a continuous irradiation with the same average dose rate and the results show practically identical behavior as far as vacancy cluster accumulation is concerned. This last result is coincident with the one obtained at a higher dose rate [15].

4. Conclusions

In this paper we have analyzed the influence of pulse and dose rate on damage accumulation and we have also made a comparison between pulse and continuous irradiation.

The conclusions we can draw are that pulse frequency shows no large effect on cluster accumulation due to the very short lifetime of interstitials relative to the pulse length and frequency, which makes the interstitial accumulation mechanism insensitive to pulse frequency.

As for vacancy clusters concentration and size, pulse repetition rate does play a role, for which we have jus-

tified the small differences appearing in the results obtained.

However, the comparison between pulsed and continuous irradiation leads to the conclusion that there is no difference concerning cluster accumulation (at 300 K and 1 Hz frequency) up to the dose reached in these simulations as long as the average dose rate is comparable. The results obtained also show good agreement with those obtained in previous work [15]. New results are needed for a higher temperature (600 K) that can strongly influence the migration and recombination dynamics.

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References

[1] T. Diaz de la Rubia, H.M. Zbib, T.A. Khraishi, B.D. Wirth, M. Victoria, M.J. Caturla, Nature 406 (2000) 871.
[2] M.J. Caturla, N. Soneda, E. Alonso, B.D. Wirth, T. Diaz de la Rubia, J.M. Perlado, J. Nucl. Mater. 276 (2000) 235.
[3] B.D. Wirth, Nucl. Instrum. and Meth. B 180 (2001) 21.
[4] T. Diaz de la Rubia, M.J. Caturla, E. Alonso, B.D. Wirth, M.A. Wall, T.A. Felter, M.J. Fluss, J.M. Perlado, in: Mathematics and Computation Reactor Physics and Environmental Analysis in Nuclear Applications, vol. 2, Senda Editorial S.A., 1999, p. 1129, ISBN 84-669.0943.
[5] B. Van der Schaaf, Fus. Eng. Des. 51&52 (2000) 43.
[6] R.W. Moir et al., Fus. Technol. 25 (1994) 5.
[7] J.M. Perlado, D. Lodi, E. Dominguez, F. Ogando, J. Prieto, T. Diaz de la Rubia, M.J. Caturla, Proceeding of 2001 MRS, San Francisco, Ca, April, 2001.
[8] J.B. Biersack, L. Haggmark, Nucl. Instrum. and Meth. 194 (1982) 93.
[9] T. Diaz de la Rubia, N. Soneda, M.J. Caturla, E. Alonso, J. Nucl. Mater. 251 (1997) 13.
[10] R. Stoller, L. Greenwood, J. Nucl. Mater. 271&272 (1999) 57.
[11] M.D. Johnson, M.J. Caturla, T. Diaz de la Rubia, Appl. Phys. Lett. 68 (1996) 57.
[12] J.M. Perlado, J. Sanz, Fus. Eng. Des. 48 (2000) 355.
[13] H. Trinkaus, J. Nucl. Mater. 296 (2001) 101.
[14] R.E. Stoller, A.F Calder, J. Nucl. Mater. 283–287 (2000) 745.
[15] E. Alonso, M.J. Caturla, T. Diaz de la Rubia, J.M. Perlado, J. Nucl. Mater. 276 (2000) 221.