# Microstructural Evolution of Electron-Irradiated Fe-Cr Alloys Using Monte Carlo Simulations

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## 1. Introduction

The development of models for estimating the mechanical stability under irradiation of steels is an important part of nuclear materials research. The international fusion materials community has focused on the development of reduced activation materials, which are based on modified ferritic/martensitic (F/M) steels. Reduced activation F/M steels are composed of Fe-Cr alloys where solute additions are included. The low-activation steels developed by the fusion program have mechanical and physical properties equivalent or superior to that of commercial steels. These steels have shown good resistance to radiation-induced swelling and helium embrittlement in experimental tests. In this paper, we investigate the tendency to form Cr-vacancy aggregates using Metropolis Monte Carlo simulations on the assumption that Fe-Cr model alloys are irradiated by electrons. It is believed that the reactions between Cr atoms and point defects account for the improved properties of Fe-Cr based alloys.

## 2. Computational Methods

In this section, we describe the simulation techniques of Metropolis Monte Carlo method. And, the interatomic potentials for Fe-Cr binary alloys are explained.

### *2.1 Metropolis Monte Carlo Method*

The Metropolis Monte Carlo (MMC) algorithm is an importance random sampling method for obtaining the thermodynamic equilibrium states of a system. In this work this method is applied to the canonical (NVT) ensemble where the number of particles (N), the system volume (V) and temperature (T) are conserved. In this ensemble, the initial number of each element – Fe, Cr, and vacancy is maintained constant throughout the simulation. The MMC simulation proceeds by randomly choosing a new trial state, based on the diffusion mechanisms. Atoms can exchange their position with neighboring vacant lattice sites or two different atoms, Fe and Cr, may rotate together. The atomic movement leads to the energy difference between the new and the previous state. For two ensemble states of $\Gamma_{old}$ and $\Gamma_{new}$, we can calculate the energy of the system before and after transition, denoted by $E(\Gamma_{old})$ and $E(\Gamma_{new})$ respectively. The new state $\Gamma_{new}$ is accepted when $\delta E$ (= $E(\Gamma_{new})$-$E(\Gamma_{old})$) is less than or equal to zero. If $\delta E$ has a positive value, the new state is accepted according to the following rule. After generating a random number $\eta$ between 0 and 1, we compare $\eta$ with the term $\xi$.

$$\xi = \exp(-\delta E / k_B T) \qquad (1)$$

where $k_B$ is the Boltzmann constant and T is the temperature. If $\xi > \eta$, then we accept the new state $\Gamma_{new}$.

The MMC can simulate a thermodynamics ensemble at the equilibrium state. Therefore, the basic assumption in this study is that the system will evolve towards the equilibrium state as the step number increases. After the specified number of Monte Carlo steps, the minimum-energy configuration of the atomic distribution is obtained. The energy difference $\delta E$ depends on the interaction model for the Fe-Cr binary alloy. The Fe-Cr potential, derived by Olsson et al., was used as an interatomic potential in this study [1].

### *2.2 Fe-Cr Interatomic Potentials*

Different types of Fe-Cr alloy potentials have been formulated using the Finnis-Sinclair approach as well as the Embedded Atom Method (EAM). In this work, we applied a two-band second-moment model which extends second-moment expression for the total energy of binary alloys with contributions from *s*-band electrons. According to the two-band modeling formalism, the energy of atom *i* is given as:

$$E_i = \frac{1}{2}\sum_j V(r_{ij}) + F_d(\rho_d) + F_s(\rho_s) \qquad (2)$$

where $V(r_{ij})$ is the pairwise electronic interaction between atoms i and j, the function $\rho_b = \sum \phi_b(r_{ij})$ represents the density of s- and d-band electrons, $F(\rho_b)$ is the many body term, and $r_{ij}$ is the scalar distance between atoms i and j. Unlike the EAM potentials, the s-band functional is included in the formalism. The details of the Fe-Cr interatomic potential are well described in Ref. [1]. The big advantage of the two-band second-moment model of

Fe-Cr is to reproduce thermodynamic properties of the alloy over the whole range of Cr concentration, including solubility limits and formation of the α-prime phase under thermal aging.

## 3. Results

We developed the lattice MMC code to investigate the interactions between vacancies and solute atoms. The presence of vacancies in the Fe-Cr alloys presupposes that those alloys are irradiated by electrons. Since the mass of electrons is not large enough to induce the displacement cascades as compared to neutrons and ions, most defects produced by electron irradiation take the form of isolated point defects, that is, single interstitials and vacancies. A vacancy is located in a box randomly and the Monte Carlo step consists of either choosing one of the eight possible first-nearest vacancy jumps or exchanging a Cr atom with one of the eight nearest-neighboring atoms. We performed the MMC calculations in 20x20x20 lattice unit boxes for the initial random distribution of Cr atoms in Fe-5Cr, Fe-9Cr, Fe-12Cr, and Fe-15Cr at T = 300K.

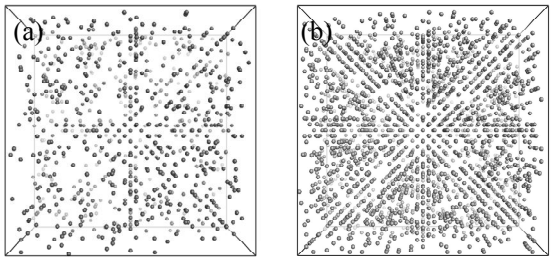


Figure 1. Spatial Cr distribution in initially random (a) Fe-5Cr and (b) Fe-15Cr aged at 300 K. No clustering of Cr atoms is dominant.

In Fig.1, the spatial distributions in initially random Fe-5Cr and Fe-15Cr are shown in the simulation box after $10^6$ trials, corresponding to one week of simulation time. No qualitative difference is observed between the initial and final states of Cr-atom distributions. Initially isolated three vacancies are included in the box, which are assumed to be generated by electron irradiation. We could not observe the clustering of Cr atoms around the vacancies. Unlike the Fe-Cu alloys, the vacancies do not play a role in the nucleation of any microstructure [2].

In order to investigate the changes of the atomic configurations in a quantitative way, the radial distribution function (RDF) was derived, which describes at which distance atoms are from each other. Fig. 2 show the MMC

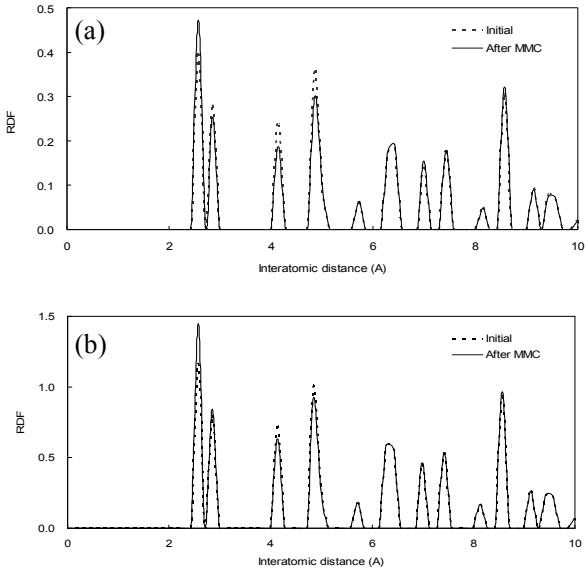


Figure 2. Cr-Cr radial distribution functions obtained from the MMC simulations of (a) Fe-5Cr and (b) Fe-15Cr alloy.

simulation results for Fe-Cr alloys. The first peak appears at 2.57Å corresponding to the first nearest-neighbor distance in a bcc lattice. We could find an increase (~20 %) of the first peaks of the RDF, which implies the tendency to form Cr clustering. The degree of clustering, however, is not dominant.

## 4. Conclusions

This paper has attempted to predict the equilibrium microstructure in Fe-Cr alloys using the Monte Carlo methods. The MMC code was developed using the Fe-Cr potentials based on the two-band second-moment model. It is found that the clustering of Cr atoms occurs but its tendency is not strong. When the isolated vacancies are present in the matrix, assuming the electron irradiation condition, the evolution of microstructure around the vacancies does not take place. Such a result might be related to the properties of swelling resistance in Fe-Cr alloys.

## REFERENCES

[1] P. Olsson, J. Wallenius, C. Domain, N. Nordlund, and L. Malerba, "Two-band modeling of a-prime phase formation in Fe-Cr", Phys. Rev. B 72, p.214119, 2005.
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