

Molecular dynamics simulations of point defect interactions in Fe–Cr alloys

K.L. Wong^a, J.H. Shim^{a,b}, B.D. Wirth^{a,*}

^a Nuclear Engineering Department, University of California, Berkeley, MC 1730, Berkeley, CA 94720-1730, USA

^b Nano-Materials Research Center, Korea Institute of Science and Technology, Seoul 136-791, Republic of Korea

Abstract

Predicting the performance of Fe–Cr ferritic martensitic steels in fusion energy environments requires an understanding of point defect properties, including the influence of solutes, impurities and other defects on their migration behavior. This paper presents molecular dynamics simulations of the effect of Cr on the diffusion of single, di- and tri-interstitials in Fe–10%Cr alloys. Two Finnis–Sinclair-type potentials were used to model the Fe–Cr alloys, which alternately describe Cr as under- or over-sized in body-centered cubic Fe. In general, the diffusivity of the single interstitials and di- and tri-interstitial clusters was reduced in the Fe–10%Cr alloys, irrespective of interatomic potential, although the underlying mechanism was different. When Cr is undersized, interstitial diffusion is retarded through a trapping mechanism associated with bound Cr-interstitial (mixed dumbbell) complexes, whereas oversized Cr atoms retard interstitial diffusion by enhancing the rotation frequency away from one-dimensionally mobile $\langle 111 \rangle$ interstitial dumbbell configurations.

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1. Introduction

Fe–Cr alloys are candidate first wall and breeder blanket materials in future fusion reactors. Radiation damage from high-energy fusion neutrons creates a large excess of point defect and point defect cluster concentrations in displacement cascades, which, in conjunction with transmutant helium and hydrogen, are ultimately responsible for microstructure evolution that can produce deleterious changes to performance-limiting properties. Thus, predicting material performance under irradiation requires an understanding of point defect properties, including

their migration and clustering behavior and any modification in this behavior as a result of interaction with solutes, impurities and other defects. In this study, molecular dynamics (MD) simulations employing two different Fe–Cr potentials are used to study the effect of 10% Cr on self-interstitial and small interstitial cluster migration.

Studies of the effect of Cr on displacement cascade evolution in Fe–Cr alloys have observed no effect on defect production [1,2]. Although no differences were observed in the absolute number of defects formed, Cr may have an influence on the migration properties of point defect clusters that can influence eventual defect fate and produce a larger effect on microstructural properties. Recent work by Terentyev [3] has demonstrated decreased interstitial diffusivity in Fe–12%Cr based on EAM

* Corresponding author. Tel.: +1 510 642 5341; fax: +1 510 643 9685.

E-mail address: bdwirth@nuc.berkeley.edu (B.D. Wirth).

Fe–Cr potentials, although the mechanistic cause was not determined.

In this work, we investigate the effect of Cr on point defect properties and microstructural evolution in irradiated Fe–Cr alloys. The initial focus is on single interstitial and small interstitial cluster transport using MD simulations. Two different Fe–Cr interaction potentials [2] were used, which show differing size effects of Cr in the body-centered cubic (BCC) Fe matrix. The next section describes the simulation method and interaction potentials, and Section 3 presents a discussion of the results of MD simulations on the effect of Cr on single, di-, and tri-interstitial diffusion in Fe–10%Cr alloys. Simulations were also performed for Fe–1%Cr alloys, although the effect of Cr at 1% concentration was minimal, and the results are not presented here.

2. Research approach

2.1. Simulation technique

Molecular dynamics simulations were performed using the MDCASK code [4] to investigate the effect of 10% Cr on the diffusivity of single, di-, and tri-interstitials. The simulation cell consisted of $50 \times 50 \times 50$ bcc unit cells ($250,000 + N$ atoms) with periodic boundary conditions and either a single, di- or tri-interstitial ($N = 1, 2, \text{ or } 3$). Pure Fe and randomly distributed ferritic alloys with 10% Cr were simulated. Single interstitials were initially oriented in the $\langle 111 \rangle$ direction; clusters of di- or tri-interstitials were inserted as parallel $\langle 111 \rangle$ dumbbells. The MD simulations were performed at temperatures from 400 to 1000 K, with additional low temperature simulations for single interstitials at 50 to 200 K. Two different cross-potentials for the Fe–Cr interaction were used, which show contrasting size effects of Cr in the Fe matrix. Simulations were conducted for 500 ps with the defect diffusivity sampled every 10 to 200 ps.

2.2. Interatomic potentials

Finnis–Sinclair-type potentials were used to describe the interatomic interactions. The Ackland potential [5] was used to describe pure Fe, and the Finnis–Sinclair potential [6] was used for Cr atom interactions. The Ackland potential correctly predicts the stability and formation energy of self-interstitial atoms in bcc Fe, although it may predict too small of an energy difference between the $\langle 110 \rangle$ and

$\langle 111 \rangle$ split-dumbbell configurations according to recent ab-initio results [7]. The diffusion and the migration mechanism of single and small self-interstitial atom clusters is well understood with the Ackland potential [8], and the goal of this project is to understand the effect of Cr on the diffusion mechanism(s) as compared to pure Fe.

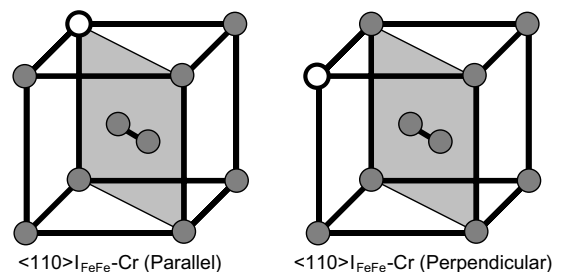
Two different Fe–Cr interaction potentials were obtained from Shim and co-workers [2], which were fit to the heat of mixing and lattice constant data using the method outlined by Konishi et al. [9]. The two cross-potentials show contrasting size effects of Cr in the Fe matrix, although both potentials predict a symmetric, positive mixing enthalpy with increasing Cr content without the negative deviation from ideality at low Cr concentrations predicted by recent ab-initio calculations [10]. The focus of this work is thus the effect of under- and over-sized Cr solute atoms on single, di- and tri-interstitial diffusivity.

The Fe–Cr I potential predicts Cr to be oversized relative to Fe, creating a compressive field around the Cr that is repulsive to neighboring Fe in the matrix. Table 1 presents the binding energies of various dumbbell–Cr configurations. Mixed dumbbells do not form readily in either $\langle 110 \rangle$ or $\langle 111 \rangle$ configuration with binding energies of -0.40 eV and -0.26 eV, respectively. A $\langle 110 \rangle$ -oriented Fe dumbbell with a Cr atom oriented perpendicular

Table 1
Binding energies of various dumbbell and Cr configurations

	Fe–Cr I	Fe–Cr II
$\langle 110 \rangle$ I _{FeCr} (Mixed)	-0.40	0.10
$\langle 111 \rangle$ I _{FeCr} (Mixed)	-0.25	0.20
$\langle 110 \rangle$ I _{FeFe} –Cr (Parallel)	-0.16	0.06
$\langle 110 \rangle$ I _{FeFe} –Cr (Perpendicular)	0.02	-0.007

All energies are given in eV. The schematic illustration below demonstrates the meaning of Cr orientations parallel and perpendicular to the axis of the $\langle 110 \rangle$ -oriented self-interstitial atom in Fe (Fe atoms represented by filled circles, while Cr is an open circle).



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