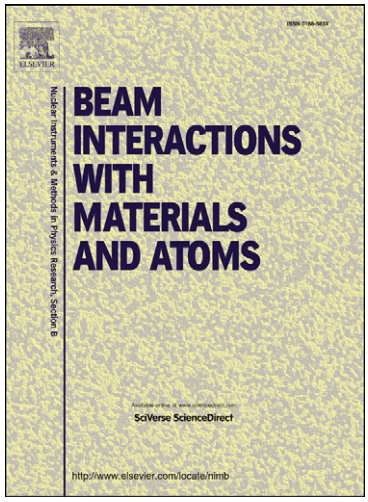

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Modelling radiation damage at grain boundaries in fcc Nickel and Ni-based alloy using Long Time Scale Dynamics Techniques

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Abstract

The long timescale evolution of radiation damage near grain boundaries (GB) in fcc Ni and a Ni-Cr alloy has been investigated. Molecular Dynamics (MD) combined with the on-the-fly Kinetic Monte Carlo (otf-KMC) has been used to study the evolution of defects in bulk, Σ3 and Σ5 GB systems resulting from 1 keV collision cascades. Results show that both interstitials and vacancies are attracted to GBs, that vacancy and interstitial clustering is observed in the bulk and vacancy clustering in the GB systems.

1. Introduction

Due to its ability to change the physical properties of materials there have been numerous studies of the effect of radiation damage on materials. One of the important effects of radiation on materials is radiation induced segregation (RIS), especially near grain boundaries (GB), as it can lead to effects such as the embrittlement of the material. Ni-based alloys represent an interesting class of materials for next generation nuclear power plants. This is due the presence of $\gamma\prime$ phase in Ni-based alloys which gives them high temperature strength and creep and oxidation resistance.

In recent years computer simulation has become an important tool to investigate such problems. MD, for instance, is an extremely powerful tool to address many problems related to radiation damage and has given insight into numerous aspects regarding radiation damage [1, 2]. The limitation of the simulation time attainable, however, means that the evolution of radiation damage cannot be simulated over realistic timescales, which drives the need for other techniques. On-the-fly kinetic Monte Carlo (otf-KMC) [3, 4, 5, 6] on the other hand allows modelling of complex systems, as it calculates the barriers at each step, and allows much longer timescales to be modelled, as it only follows diffusion events. Therefore using MD to model the initial phase of a collision cascade followed by otf-KMC to model the subsequent diffusion of defects is an extremely powerful tool for modelling the long time evolution of cascades.

Overall there is a large body of work aimed understanding the effect of radiation on Ni-based materials especially at grain boundaries [7]. Microstructure evolution in irradiated austenitic Fe-Cr-Ni has also been studied [8]. The study of RIS in this work showed enrichment of Ni and depletion of Cr at grain boundaries.

In this work we study the diffusion of vacancies near GBs and the evolution of defects after 1 keV collision cascades in bulk, Σ3 and Σ5 GB systems for the fcc Ni and a Ni-Cr binary alloy.

2. Method

Fcc Ni and a Ni-Cr binary alloy (80 at% Ni 20 at% Cr) have been studied in this work. The bulk, symmetrical tilt Σ5 and Σ3 grain boundaries have been studied for both materials. Systems modelled contained approximately 55k atoms with periodic boundary conditions in 3 dimensions for the bulk system and in the plane of GB with the top few layers fixed on the edges parallel to the GB for the GB systems. The GB systems were fully relaxed including allowing translations in the x, y and z directions to minimize the grain boundary energy. For the GBs in Ni-Cr, the minimum-energy GB in pure Ni is found first and then the required percentage of Cr is distributed randomly in the system. The system is relaxed after that holding GB separation fixed.

The Mishin 2004 [9] potential has been used to describe Ni-Ni interactions, The Olsson 2005 [10] potential for Cr-Cr interactions and Giovanni 2010 [11] potential has been used to represent Ni-Cr interactions. The three potentials have been splined to the ZBL potential [12] to correctly describe small atomic separations. The cutoff distances used to connect the pair potential to the spline function and the spline function to the ZBL potential are: 0.6 Å and 1.2 Å for Ni-Ni, 0.5 Å and 1.2 Å for Cr-Cr, 0.8 Å and 1.95 Å for Ni-Cr potential.

The modelling carried out can be divided to two main stages. The first stage was modelling collision cascades to the system and the second stage was modelling the evolution of the defects that resulted from the first stage.

Collision cascades are initialized by imparting kinetic energy to an atom, called the primary knock-on atom (PKA), in a certain direction. An energy of 1 keV was used to perform the collision cascades. The PKA has been chosen randomly and in case of the GB the direction of the collision cascades has been directed towards the GB. The initial collision cascade phase is

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