

A first principle study on the composition deviation of Ni-Si precipitates formed in irradiated stainless steel

*Dongyue CHEN¹, Kenta MURAKAMI², Naoto SEKIMURA¹

¹The University of Tokyo, Department of Nuclear Engineering and Management, School of Engineering

²The University of Tokyo, Nuclear Professional School, School of Engineering

The composition of Ni-Si precipitates formed in irradiated stainless steel was previously found to be deviated from the standard γ' phase stoichiometry by atom probe. Here a first principle calculation is attempted to explain this composition deviation by considering the possible defects in the γ' phase.

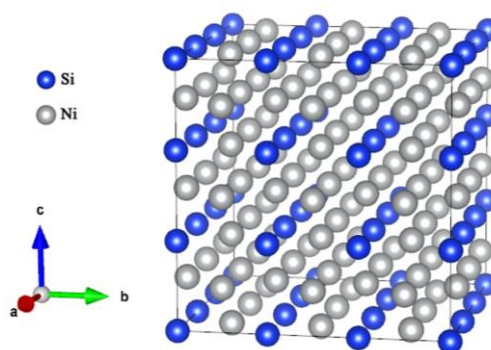
Keywords: Stainless steel, Ni-Si precipitates, First principle calculation

1. Introduction

Ni-Si precipitates will form in austenite stainless steels when they are irradiated to high dose in reactor, which threatens reactor structural integrity. The formation of these precipitates is believed to be closely related to radiation induced segregation and stress fields near sinks, which could be characterized by atom probe tomography (APT) and transmission electron microscopy (TEM), respectively. However, in our previous work, the Ni-Si precipitates observed in APT have a distinctly smaller Ni/Si atom ratio than the standard γ' phase (Ni_3Si) which was previously identified by TEM [1]. This suggests the complicated nature of Ni-Si precipitates. A proper interpretation of the experimental results is desired before APT and TEM can be combined and fully utilized for Ni-Si precipitate study. One possibility is that the lattice defects in γ' phase have caused the precipitate composition deviation, and it is verified by first principle calculation in this work.

2. Computation details

The first principle calculation is carried out by using the Vienna ab initio simulation package (VASP) [2] with the Perdew and Wang generalized gradient approximation (GGA-PW91) and the projected augment waves (PAW) method. A 108-atom $3a_0 \times 3a_0 \times 3a_0$ supercell of the γ' phase is constructed.



A 108-atom supercell of perfect γ' phase set up in VASP calculation

3. Results and Conclusions

First, the perfect γ' phase without defects is modelled. The proper lattice constant is obtained by enabling supercell volume change during relaxation. Our results of the perfect γ' phase is compared with previous phase diagram calculations, and a good match in phase formation energy and lattice constant is found. Then, one step further, different kinds of single defects are added into the perfect lattice of γ' phase, namely vacancies, dumbbells and substitutions. Among all the configurations calculated here, the defect formation energy is the lowest when one Ni atom is substituted by one Si atom. It means this configuration is thermodynamically preferred in the γ' phase. Such substitution will lead to increased Si concentration and decreased Ni concentration in the Ni-Si precipitates, and could be one reason for the smaller Ni/Si atom ratio observed in our previous APT results [1].

[1] D. Y. Chen, K. Murakami, K. Dohi et al., Annual Meeting of Atomic Energy Society of Japan, 2015, Hitachi, Japan.

[2] G. Kresse and J. Hafner, Phys Rev B Condens Matter, 1993. 47(1): p. 558-561.