STRESS INTENSITY EFFECT ON SOLID STATE OXIDATION OF Ni-Cr ALLOY WITH DIFFERENT CHROMIUM CONCENTENTS

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1. Background

The life extension of aging nuclear power plant is a challenge due to the influence of various factors on the materials properties. Ni-base alloys are widely used in light water reactor component and stress corrosion cracking (SCC) has been found in pressurized water reactor (PWR) components such as vessel head penetrations and bottom mounted instrument nozzles fabricated with Alloy 600 and its weld metals [1,2]. Ni-base alloys composed of several elements among them nickel and chromium are the major ingredients. X-ray photoelectron spectroscopy (XPS) study of Ni-Cr alloy examined that Cr is oxidized preferentially to Cr$_2$O$_3$ initially but that Ni in the alloy is oxidized more rapidly to NiO than Ni metal [3]. Alloy 600 XPS study found the chromite-rich inner layer due to inward oxygen penetration and simultaneously with outward migration of nickel [4]. However, some theoretical and experimental studies have been carried out on Ni/H$_2$O and oxygen preadsorbed Ni/H$_2$O to understand water dissociation and adsorption phenomena [5,6]. Over the years various attempts have been made to obtain mechanism of SCC but it still require more fundamental study to interpret clearly. This study presents an approach based on the multiscale modeling, to assess the influence of alloy composition and stress intensity (K) on the initial stage solid state oxidation of the Ni-Cr binary alloy. The multiscale modeling considers different length scales such as finite element method (FEM) – quasi-continuum (QC)-quantum chemical molecular dynamics (QCMD), for analyzing crack tip molecular domain.

2. Computational Methods

Multiscale method is a newly developed tool to analyze materials issue. It is an important part of the multiscale modeling to make linkage in between different scales. SCC is a difficult task to assign multiscale methods from atom to component. We have applied a hierarchical computational model that consist of three different methods to simulate initial stage of oxidation for SCC problem. The details about this method can be seen elsewhere [7]. The crack tip is a few nanometer wide and chemical reaction is being performed by tight-binding QCMD. This region plays an essential role for primary stage SCC initiation. The slab models for this method is consisted of 48 metallic atoms consider an average size model with single layer six water molecules placed on surface. We have substituted different chromium (10, 15 and 20 percentages) atoms in the Ni surface with or without applying stress intensity. The initial structure for this calculation is shown in Fig. 1. Total number of simulation step was 5000 where each step was 0.2 femtosecond (fs) with the Verlet algorithm. The ensemble for this simulation...
Figure 1 Ni-Cr (111) initial surfaces with different chromium concentration (a) 10%, (b) 15% and (c) 20%

was constant volume and constant temperature (NVT) and the temperature is controlled by using scaling the atom velocities. Temperature was considered 598 K for PWR condition and pressure was atmospheric.

3. Results and Discussion

The interaction of water with a metal surface is of fundamental interest in studying catalysis, corrosion and passivation phenomena. There are several studies discussed about water absorption on metal surface whether molecularly or dissociatively absorbed [8-10]. However, Pache et al. have demonstrated that water adsorbs molecularly on nickel surface up to 260 K [11]. In PWR environment, metal water interaction resulted in dissociation of water molecules. Water molecules moved towards the metal surface with progressing of reaction. After a few hundreds of fs, the interaction assisted to dissociate water molecules into OH, H or O. Subsequently, dissociated hydrogen diffused quickly in the surfaces through the interstitial hollow sites due small atomic size. Some of the hydrogen remain above the surface that can dissolve into the solution. Oxygen atoms penetrate metal surfaces quite slowly as compared to hydrogen. Figure 2 shows the various kinds of simulated surface morphologies. The oxygen concentration is significantly high around the chromium and it indicates the initiation of passivation. Chromium
4. Conclusions

The stress intensity effect on initial stage oxidation of Ni-Cr(111) binary alloy surface has been studied by multiscale modelling. QCMD method has applied to analyze reaction dynamics at the crack tip molecular domain. FEM have employed to find the stress intensity effect on CT specimen crack tip at micro level and the micro zone has prepared for the QC model. After the completion of QC calculations, obtained atomic positions in the deformed crystal structure are used to construct for oxidation mechanism analysis. The QCMD simulated results examined that the chromium segregated faster than nickel atoms and make preferential bonding with oxygen. The preferential bonding originates a passive film formation. Applied stress intensity deformed the structure which may increase the atomic distance. This distance heighten the absorbtion of water molecule or OH or oxygen into lattice. Substitution of chromium into the surface decelerates oxygen diffisivity due to surface passivation. In conclusion, the stress intensity raise the crack tip solid state oxidation that may enhance at the beginning stage of SCC initiation.


