An Integrated Study on a Novel High Temperature High Entropy Alloy

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Outline

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Introduction

- Project Period: 10/1/2013 --- 9/30/2015
- Project Manager: Steven Markovich
- Project Objectives:

(1). Perform molecular dynamics (MD)/Monte Carlo (MC) and interface energy HPC simulation on the HEA models to screen out the potential high temperature and high pressure oxidation resistant and low temperature ductile ODS HEA candidates.

(2). Perform experiments on the high temperature and high pressure property of the most promising ODS HEA systems from the simulation.

(3). Train students and postdocs.

Introduction

1. The high temperature high entropy alloys (HEAs), such as NbMoTaW and TaNbHfZrTi, show considerable promise to have higher operating temperature, good mechanical properties at high temperature, major improvement in high temperature oxidation resistance and structure stability.

2. The recent development of molybdenum (Mo) alloys, with nano-scale powders of transition metal oxides (La_2O_3) that sparsely dispersed in the Mo matrix named oxide dispersion strengthened (ODS) alloy, giving over 800 MPa yield strength and ~40% room temperature tensile elongation, is based on the idea that impurities within the crystal can act as pinning centers for dislocations.

3. To save time and expense, we need integrate computation with experiment to avoid triae.

Methods We Used

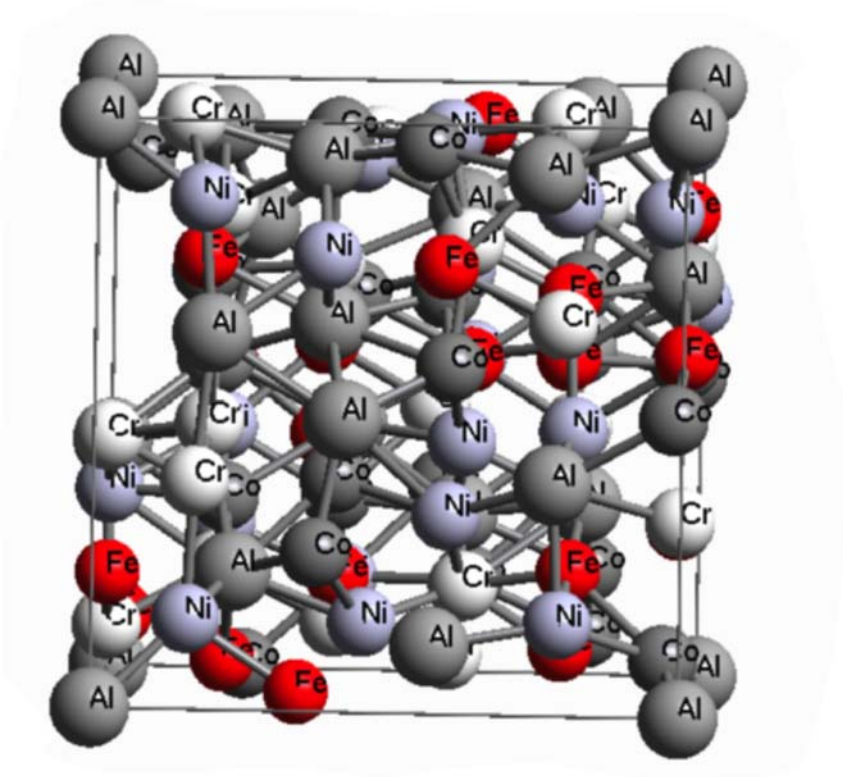
1. Perform *ab initio* density functional theory (DFT) method based molecular dynamics (MD) and long time Monte Carlo HPC simulations on the high temperature and high pressure behavior of the potential candidate ODS HEAs. The interface energies and bonding of different dopant elements and concentrations will be compared and optimized to obtain the most stable structure.

2. Experimentally validate the predicted potential high performance high temperature HEAs. High temperature oxidation, corrosion, and microscopy tests will be performed at locally. Special in-situ high pressure tests on the new materials will be performed at Lawrence Berkeley National Laboratory (LBNL) Beamline 12.2.2.

Current Status and Preliminary Results

1. We had started simulation on two HEAs: AlxFeCoCrNi and NbHfZrMoTaTi;
2. We had performed synchrotron XRD compress and decompress experiment on the AlxFeCoCrNi and NbHfZrMoTaTi.
3. We started the computational material design training.

Simulation Results: AlFeCoCrNi

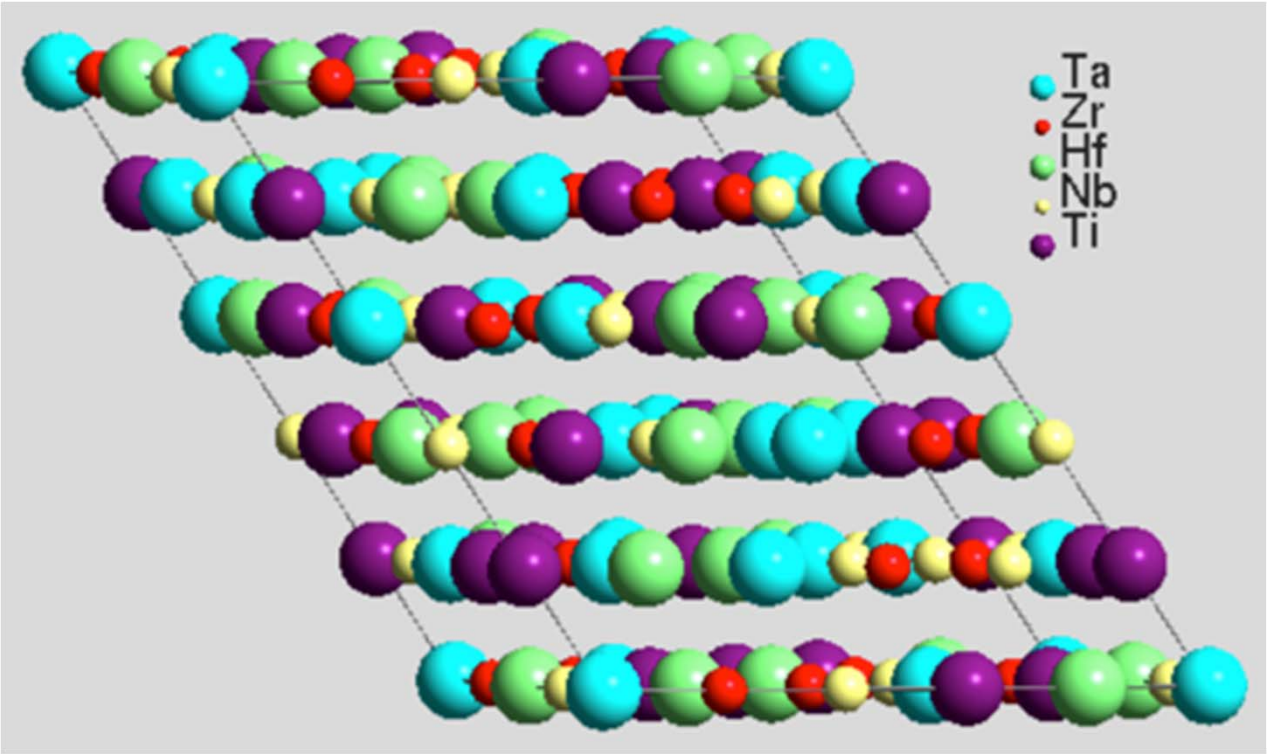


The optimized AlFeCoCrNi crystal structure with 20 Al, Fe, Co, Cr, Ni atoms each in the unit cell.

Simulation Results: AlFeCoCrNi

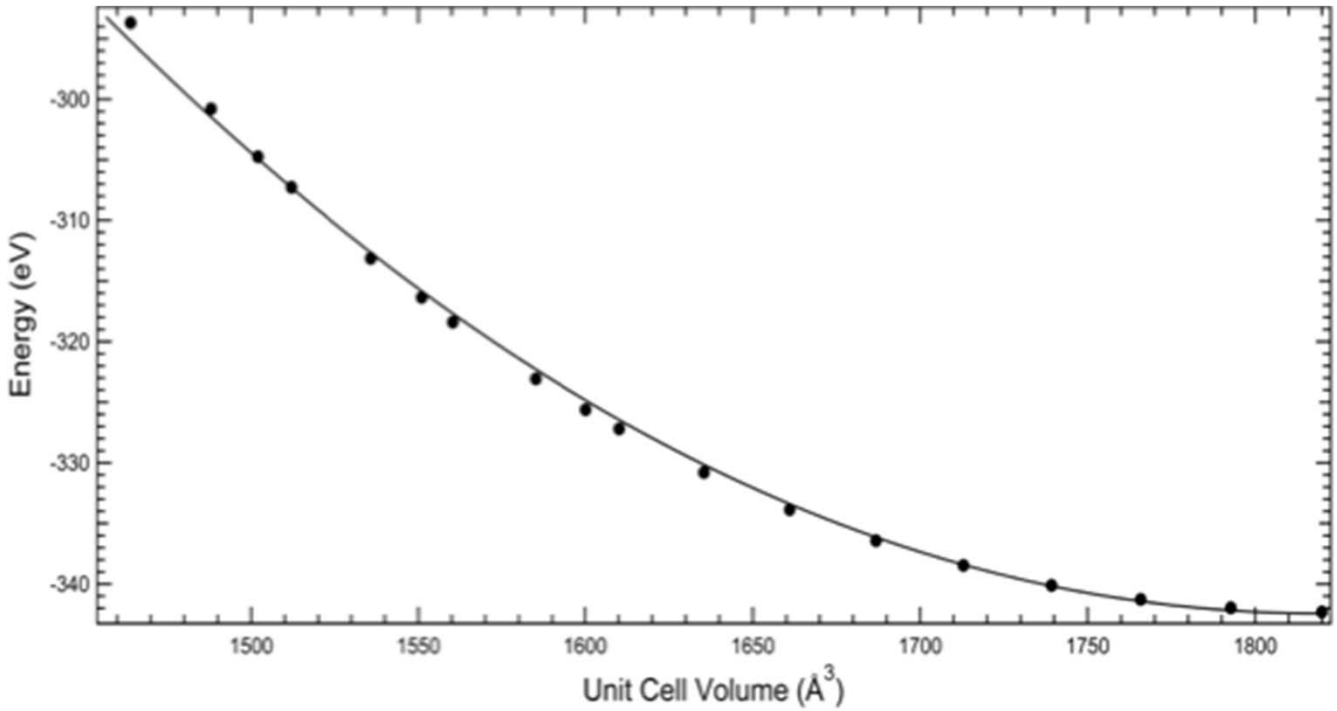
We have been using VASP codes (MedeA package) to efficiently optimize and predict possible stable HEA structures. In our VASP simulation, we performed the *ab initio* density functional theory (DFT) based electronic structure simulations and optimized the AlFeCoCrNi crystal structure. The local density approximation (LDA) was used with 400 eV plane wave energy cutoff. The energy convergence was set to be less than 0.01 meV while the force convergence was set at less than 0.2 meV/Å.

Simulation Results: NbHfZrTaTi



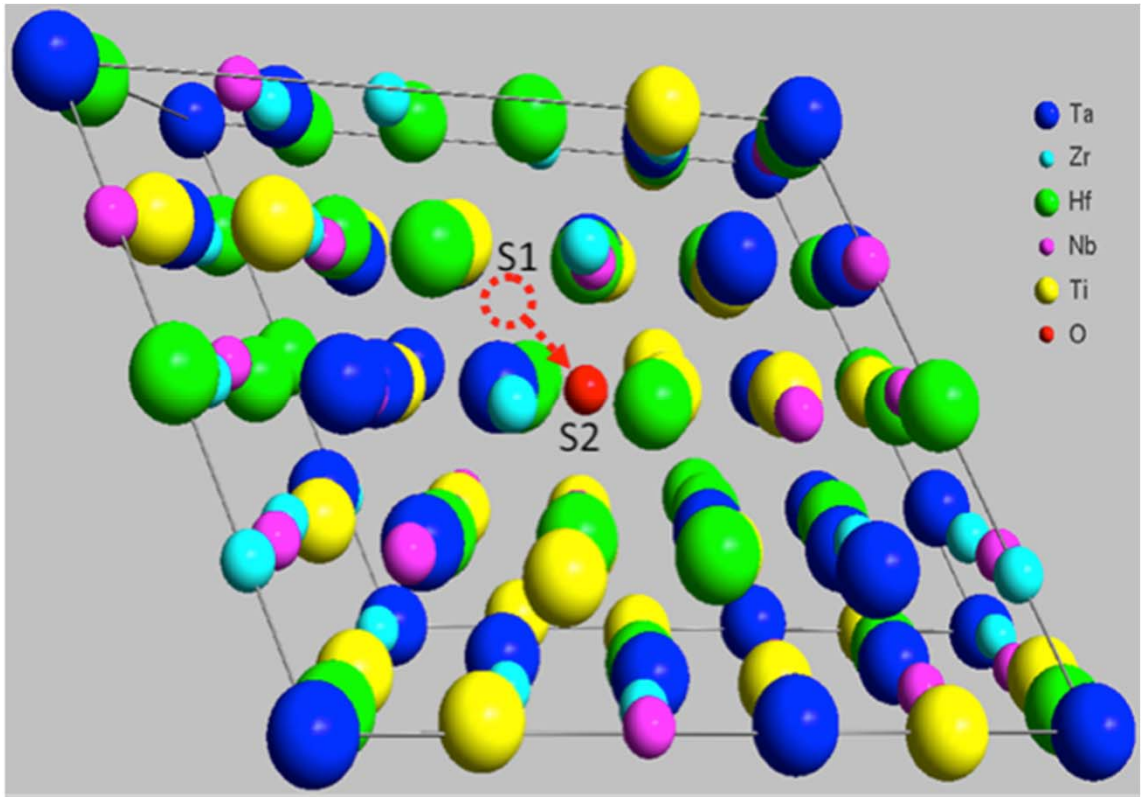
The model will be used in simulation for NbHfZrTaTi.

Simulation Results



The black dot - compression data.
The best fit solid line of the Birch–Murnaghan equation.
The bulk modulus 198 Gpa.

Oxygen Diffusion Simulation: NbHfZrTaTi

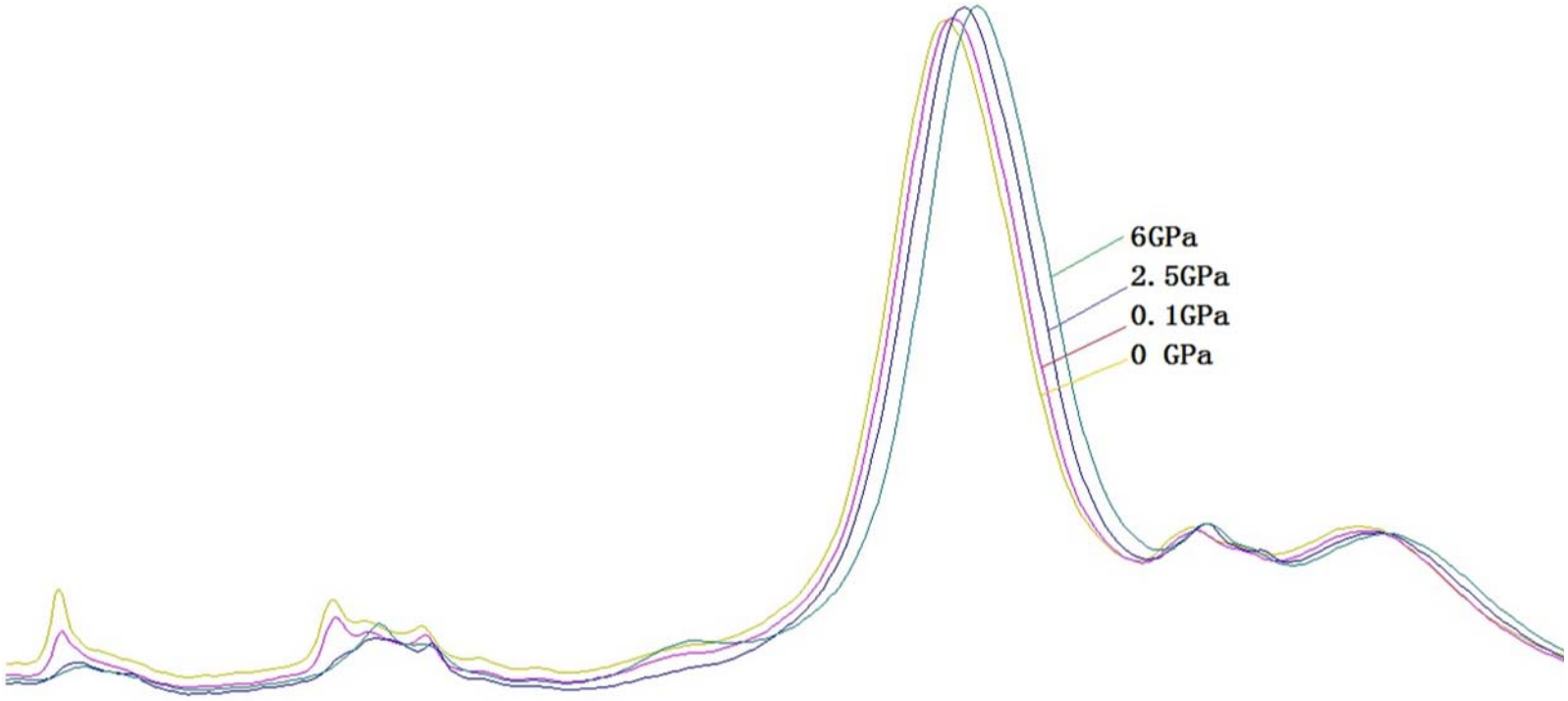


Model of HEA TaNbHfZrTi for vacancy formation energy calculation.

Oxidation Simulation Results

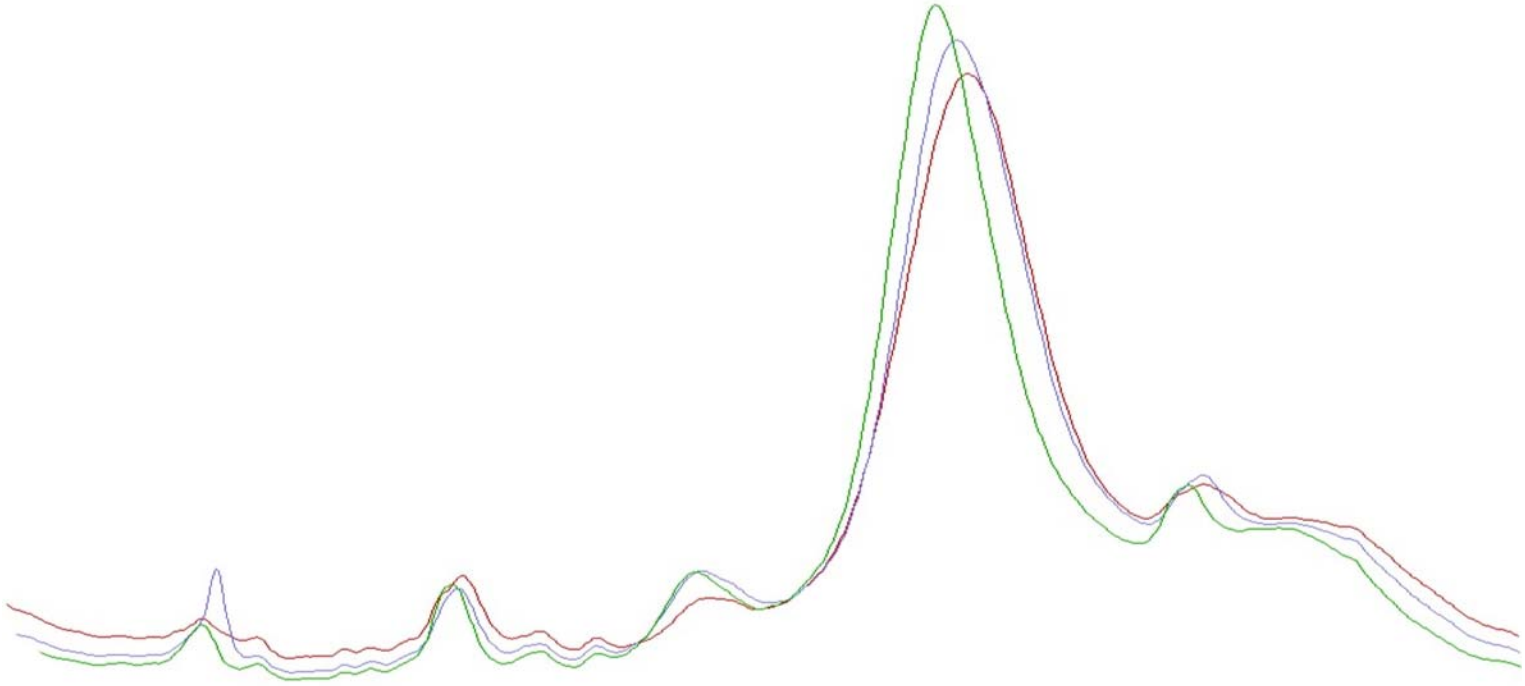
- The nudged elastic band (NEB) method in VASP is used to investigate the alloy's oxygen diffusion barrier.
- The average diffusion barrier is at ~ 0.2 ~0.5 eV higher than those of pure Nb, which is ~1.2 eV.

Synchrotron XRD Results: AlFeCoCrNi Compression



The synchrotron XRD results of AlFeCoCrNi compression.

Synchrotron XRD Results: AlFeCoCrNi Decompression



The synchrotron XRD results of AlFeCoCrNi decompression.

Synchrotron XRD Results: AlFeCoCrNi

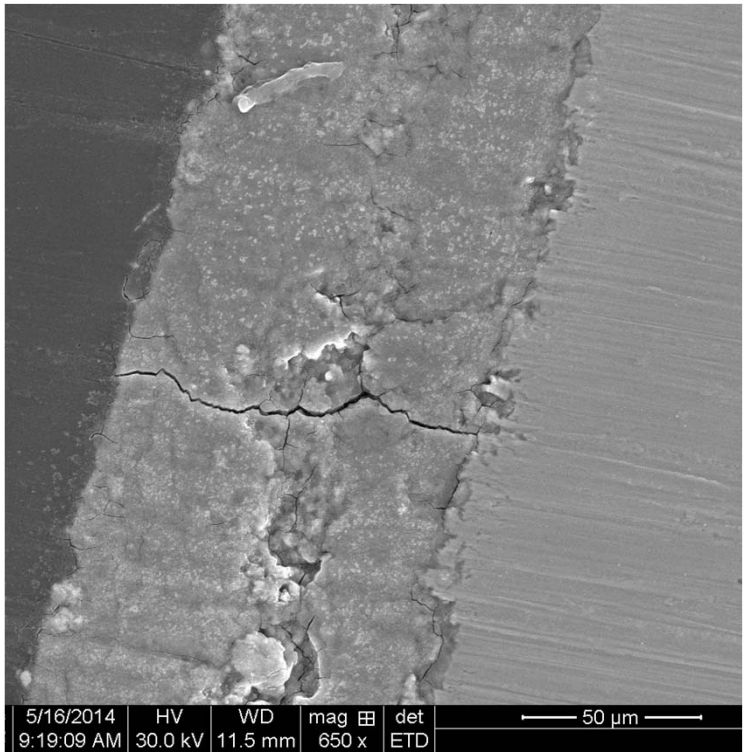
Our preliminary compress and decompress XRD data shows that the crystal structure is very stable up to ~ 25 GPa and decompress to ambient pressure. The MoHfZrNbTaTi data processing is ongoing.

$Al_xFeCoCrNi$ Hot Corrosion

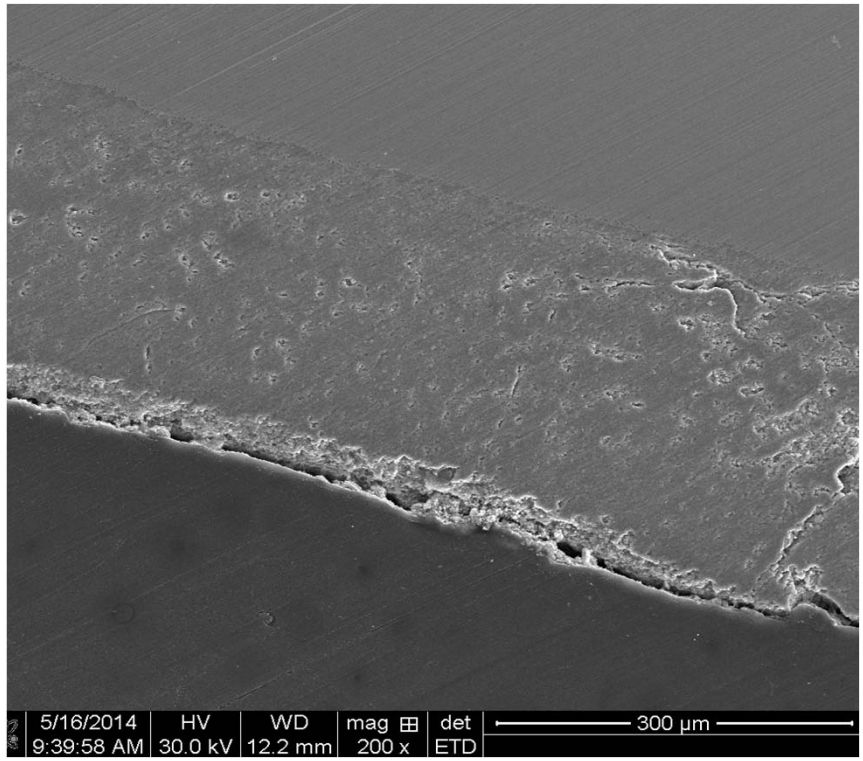
1. Different compositions of Al HEA samples $Al_xFeCoCrNi$ in the presence of molten mixture of $Na_2SO_4+V_2O_5$ (50% : 50%) at 900 ^oC were tested.

2. Hot corrosion in 2 cycles 8 hours.

$Al_xFeCoCrNi$ Hot Corrosion

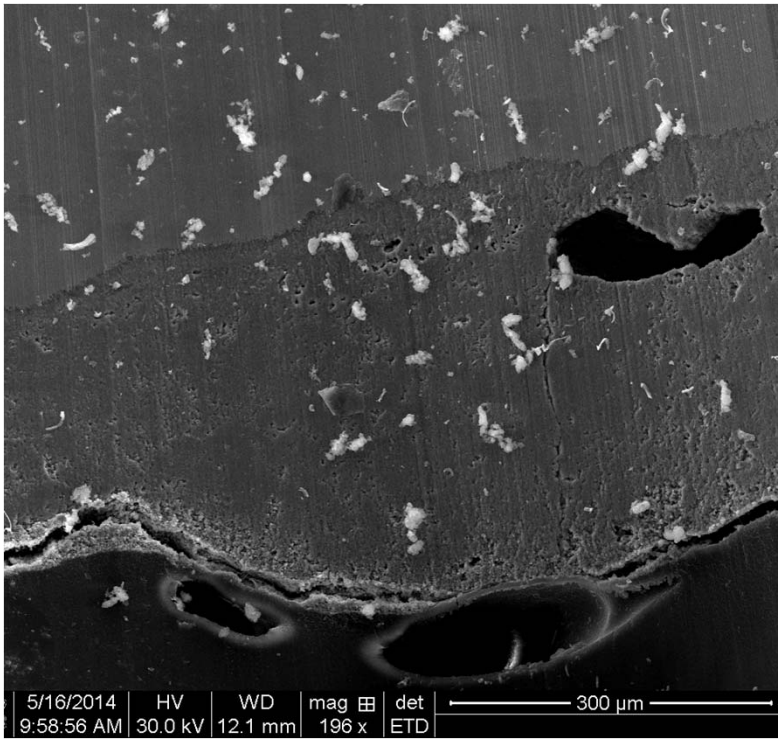


$Al_{0.3}FeCoCrNi$ hot corrosion

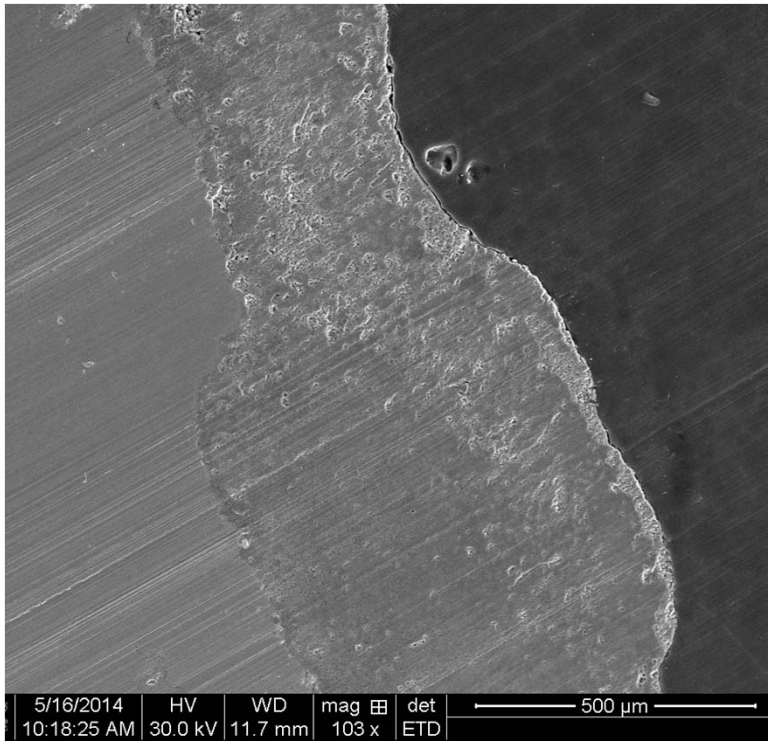


$Al_{1.0}FeCoCrNi$ hot corrosion

$Al_xFeCoCrNi$ Hot Corrosion



$Al_{1.5}FeCoCrNi$ hot corrosion



$Al_{2.0}FeCoCrNi$ hot corrosion

$Al_xFeCoCrNi$ Hot Corrosion

1. $Al_{0.3}FeCoCrNi$ hot corrosion has the thinnest corrosion layer;
2. $Al_{2.0}FeCoCrNi$ hot corrosion has the thickest corrosion layer;
3. Longer time hot corrosion tests are ongoing;
4. $Al_{1.0}FeCoCrNi$ has better room temperature ductility.

Future Work

1. Continue to screen the interface models and perform *ab initio* HPC simulation to study the high temperature corrosion and low temperature ductility. The microstructures, elastic constants, and diffusion property will also be simulated.

2. Experimentally validate the predicted ODS HEAs: synthesize samples and characterize the high temperature and low temperature properties.

3. Students and postdocs training on ODS HEA simulation and validation.

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