

Novel Nano-size Oxide Dispersion Strengthened Steels Development through Computational and Experimental Study

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Outline

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Introduction

- Project Period: 6/1/2012 --- 5/31/2015
- Project Manager: Maria M. Reidpath and Vito Cedro
- Project Objectives:
 - (1). Perform interface energy and molecular dynamics/Monte Carlo HPC simulation on the ODS models to screen out the potential high temperature and high pressure ODS candidates.
 - (2). Perform experiments on the high temperature and high pressure property of the most promising ODS systems from the simulation.
 - (3). Students/postdocs training.

Introduction

1. The oxide dispersion strengthened (ODS) steel alloys have higher operating temperature, major improvement in high temperature oxidation and dislocation creep resistance.
2. The recent development of ODS alloys with nano-scale powders of transition metal oxides (Yttrium and Chromium) that dispersed in the matrix is based on the idea that impurities within the crystal can act as pinning centers for dislocations.
3. The ODS FeCrAl alloys have been demonstrated having unique properties at temperature up to 1200 °C.
4. Under high pressure, the current study on the dislocation creep resistance improvement at high temperature is limited to the trial and error method which is expensive and time consuming.

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 ODSs. 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 alloys. 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 Achievements

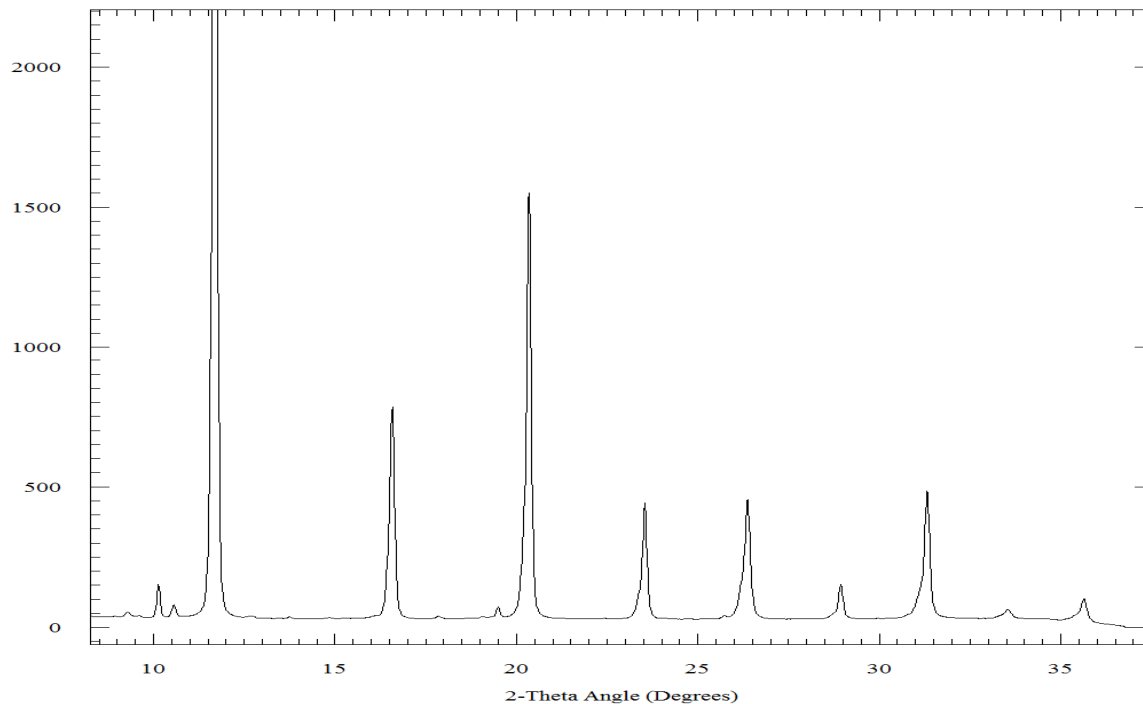
1. The MA956 samples with 20% Cr 4.5 % Al, 0.5 Ti, 0.5% Y_2O_3 and balance Fe were tested. The test results provides info for a good Fe/YTiCrAlO simulation models.

As a model high pressure experimental system, the pure Ni and NiS samples were tested with high pressure radial synchrotron XRD. The grain rotation of Pt in Ni media was detected. The NiS results show that the S concentration increase from 7% to 20% makes the NiS brittle.

ODS XRD Results

- We have synthesized the ODS with Cr: 20%, Al: 4.5%, Ti: 0.5%, Y_2O_3 : 0.5% and Fe balance ratio by low temperature ball milling. SPEX 8000 mixer was used with Ar gas protection and liquid nitrogen cooling.
- The major XRD 8 peaks are from BCC Fe. The strongest XRD peak is from BCC Fe (110). The rest small peaks are from the XRD of Cr, Al, and Y_2O_3 .

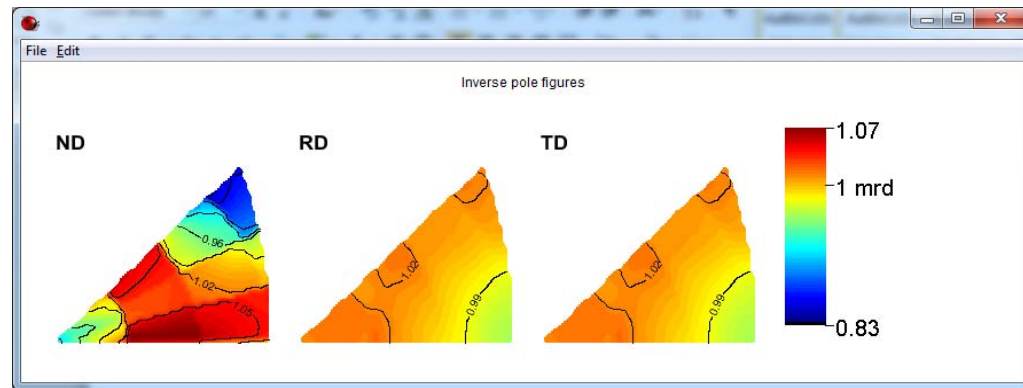
The ambient pressure XRD result



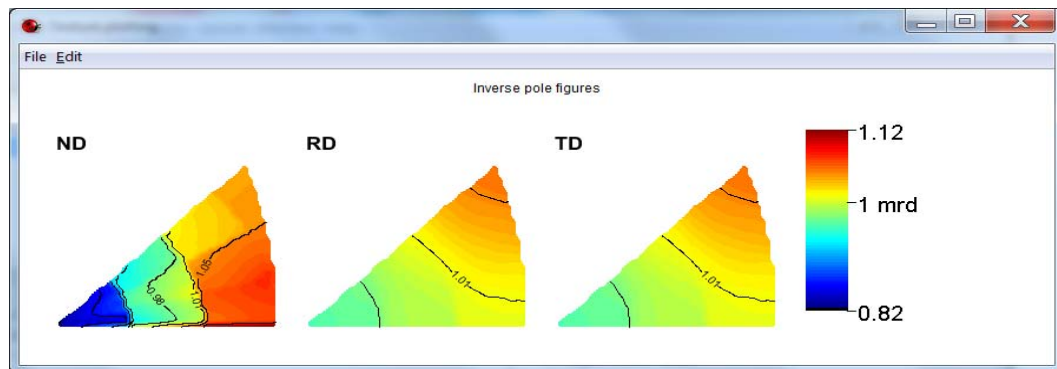
- The ambient pressure XRD result with Cr: 20%, Al: 4.5%, Ti: 0.5%, Y_2O_3 : 0.5%, and balance Fe.

NiS Texture Results

- 7% NiS (0.5GPa)

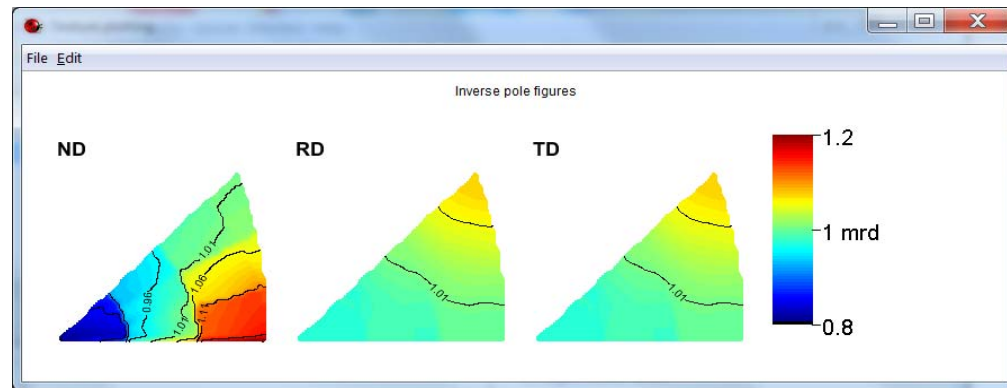


- 7% NiS (24.5GPa)



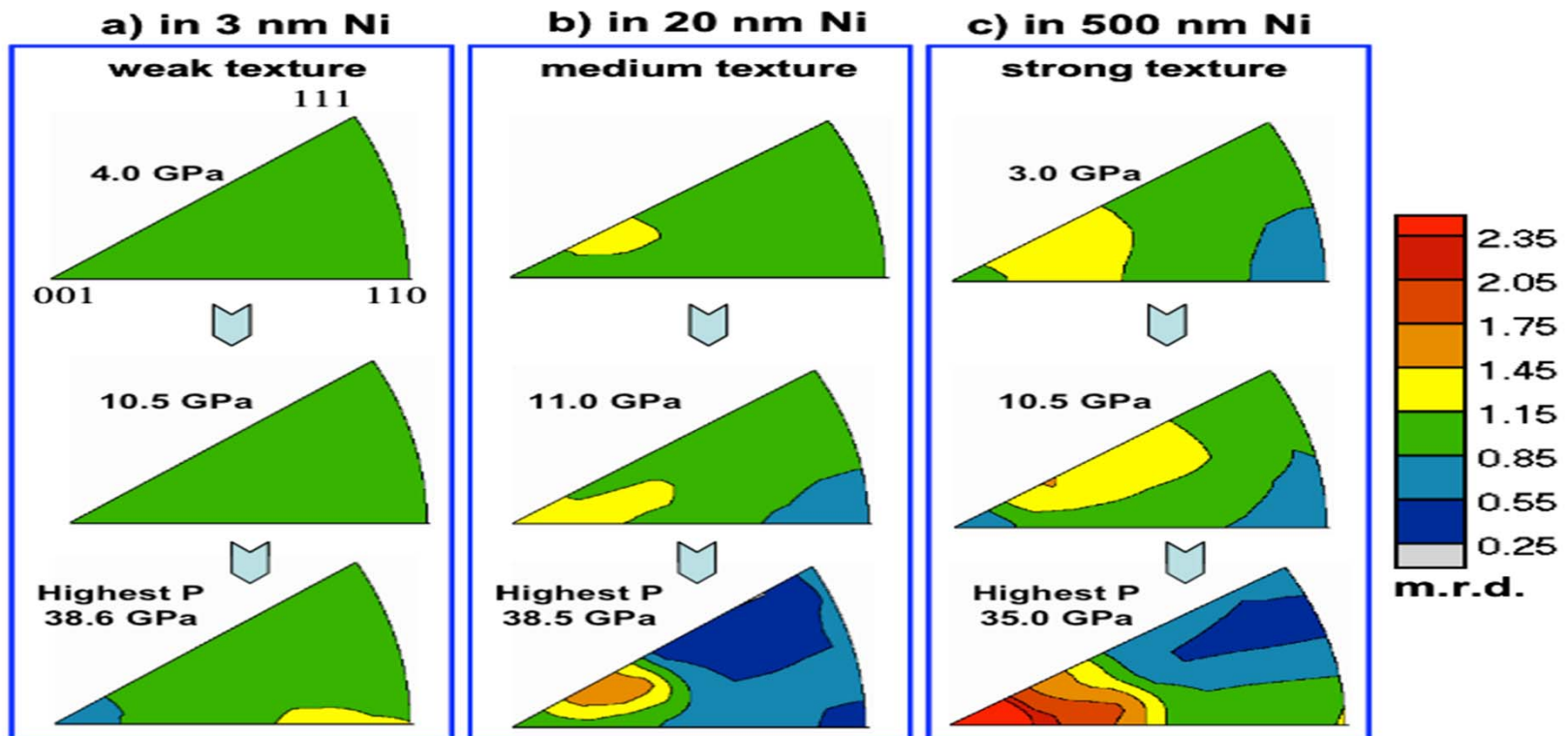
NiS Texture Results

- 14% NiS (0.5GPa)



- Our synchrotron XRD radial compress and decompress experiment data clearly shows that 14% S doped Ni becomes brittle when the S concentration reaches 14% while in 7% it is ductile.

Grain Rotation Detection



Inverse pole figures of platinum in 3 nm (a), 20 nm (b), and 500 nm (c) nickel media along the compression direction (normal direction).

Grain Rotation Detection

In fine nanocrystals, much higher shear stress is needed for the nucleation of dislocations. Dislocations play little in equilibrating the system. Instead, grains rotate to minimize the compression induced energy increase. Therefore, fine nanocrystals have higher rotation rate. The grain rotation of nickel nanocrystals leads to rotation of neighboring platinum particles. The orientations of platinum particles are hence changed, which results in the loss of texture.

Current Status and Results

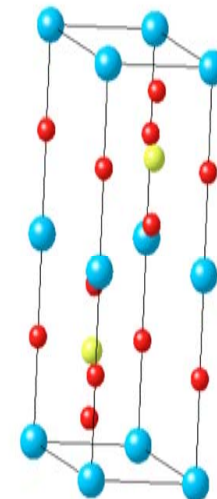
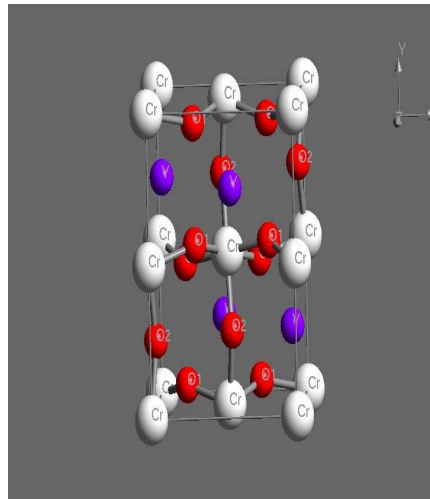
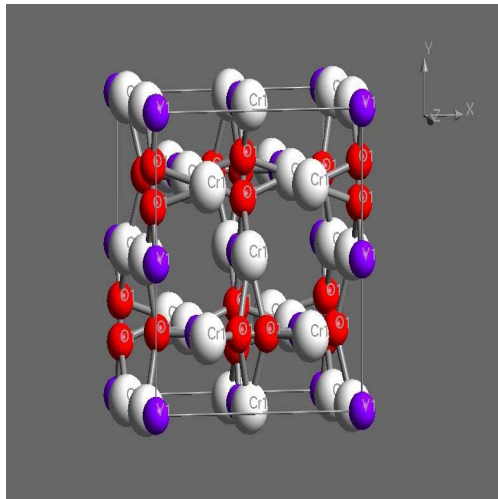
2. The interface compounds YCrO_4 , YCrO_3 , and YAlO_3 were simulated by *ab initio* density functional theory method.

We took the plane wave cutoff energy as 400 eV and spin polarized simulation was performed.

The bandgap of YCrO_3 at Gamma point is 0.48 eV while for YCrO_4 this is 0.31 eV, which are semiconductors. For YAlO_3 (P6_3mmc and Pnma) this is 5.91 eV and 6.62 eV, which are insulators.

The phonon calculations show that the main difference between YCrO_3 supercell and YCrO_4 supercell phonon dispersion curves is in YCrO_3 supercell phonon dispersion curve, there is an extra high frequency phonon band from 25 THz ~ 28 THz while in YCrO_3 supercell curve the phonon is continuous from 0 ~ 17 THz.

YCrO_3 , YCrO_4 , and YAlO_3 Simulation



YCrO_4 , YCrO_3 , and YAlO_3 structures used in our simulation. All have rectangular structures. The purple/yellow balls stand for Y atoms, white/blue balls for Cr/Al atoms while red balls for O atoms.

YCrO₃ Elastic Constants

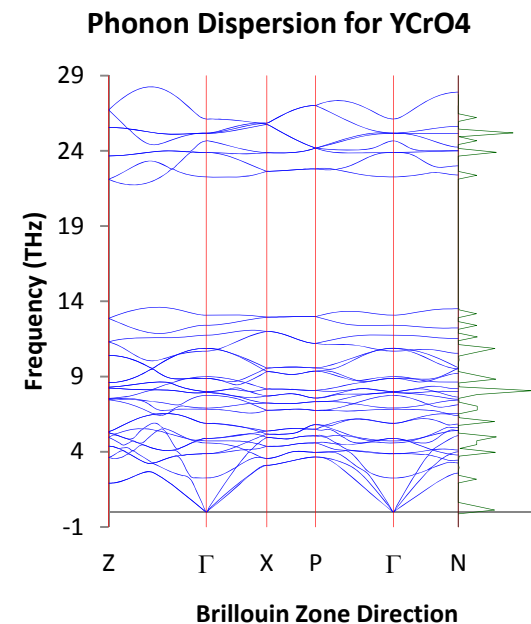
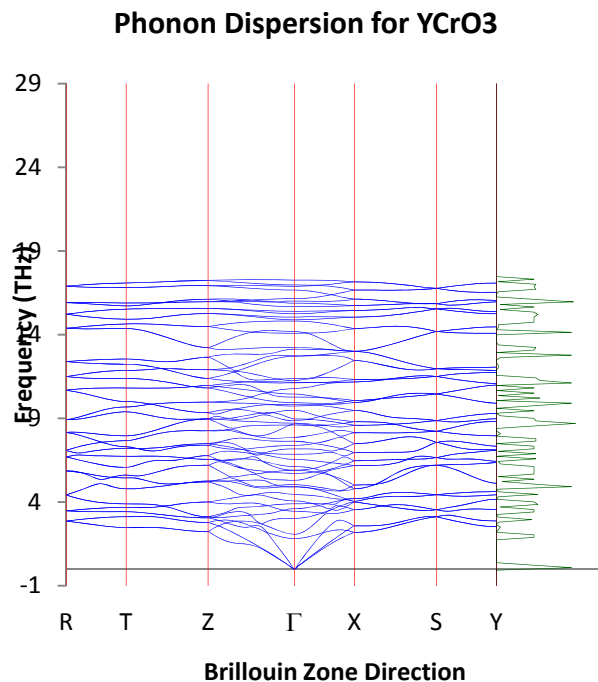
Modulus	Voigt	Reuss	Hill
Bulk	189.91	189.52	189.72 GPa
Shear	99.13	95.25	97.19
Young's	253.31	244.75	249.03
Longitudinal			319.30

Velocity of sound

transverse waves:	3972 m/s
longitudinal waves:	7200 m/s
mean:	4427 m/s

Debye temperature: 608.0 K

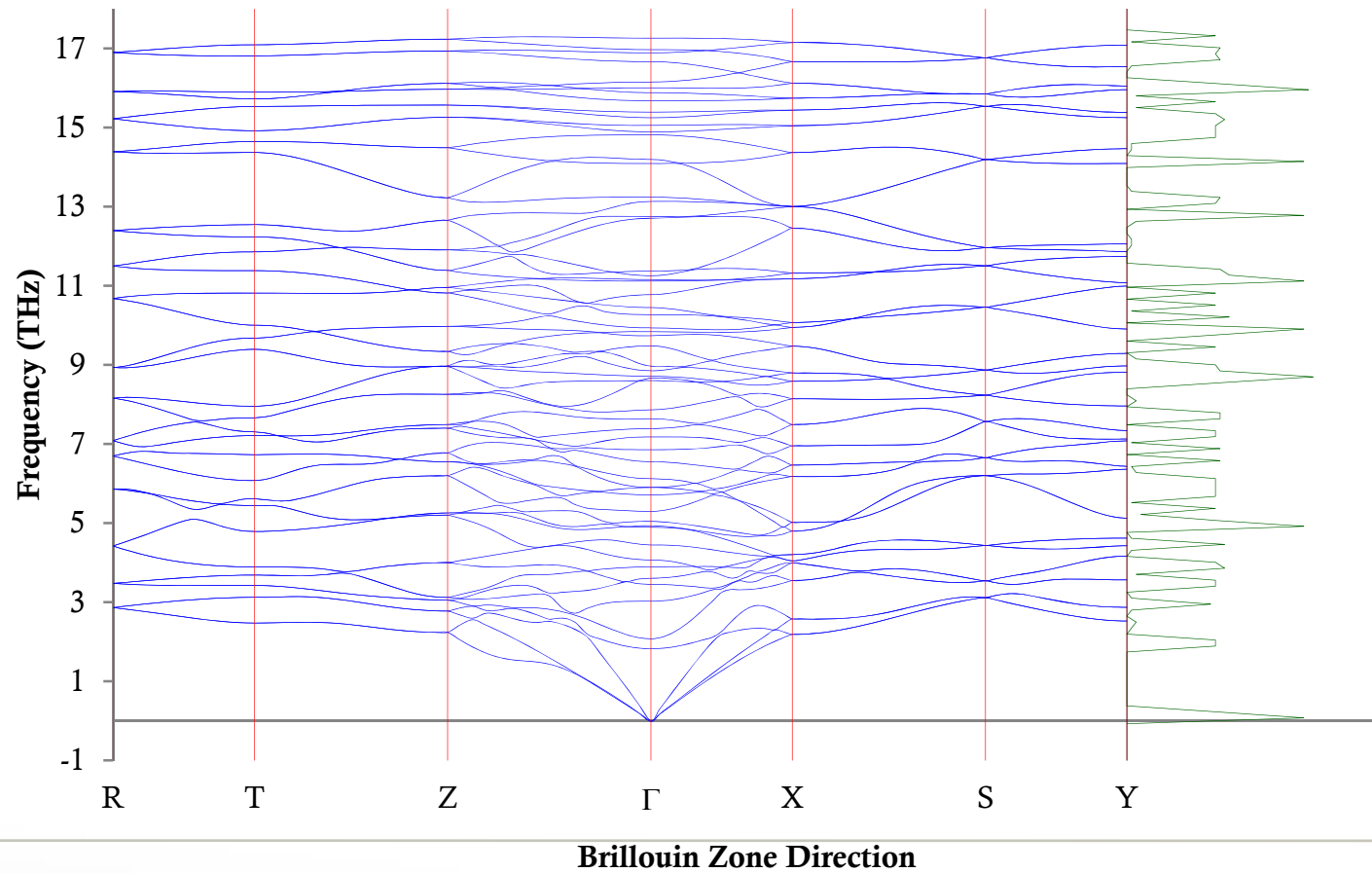
YCrO₃ and YCrO₄ Phonon Dispersion and DOS



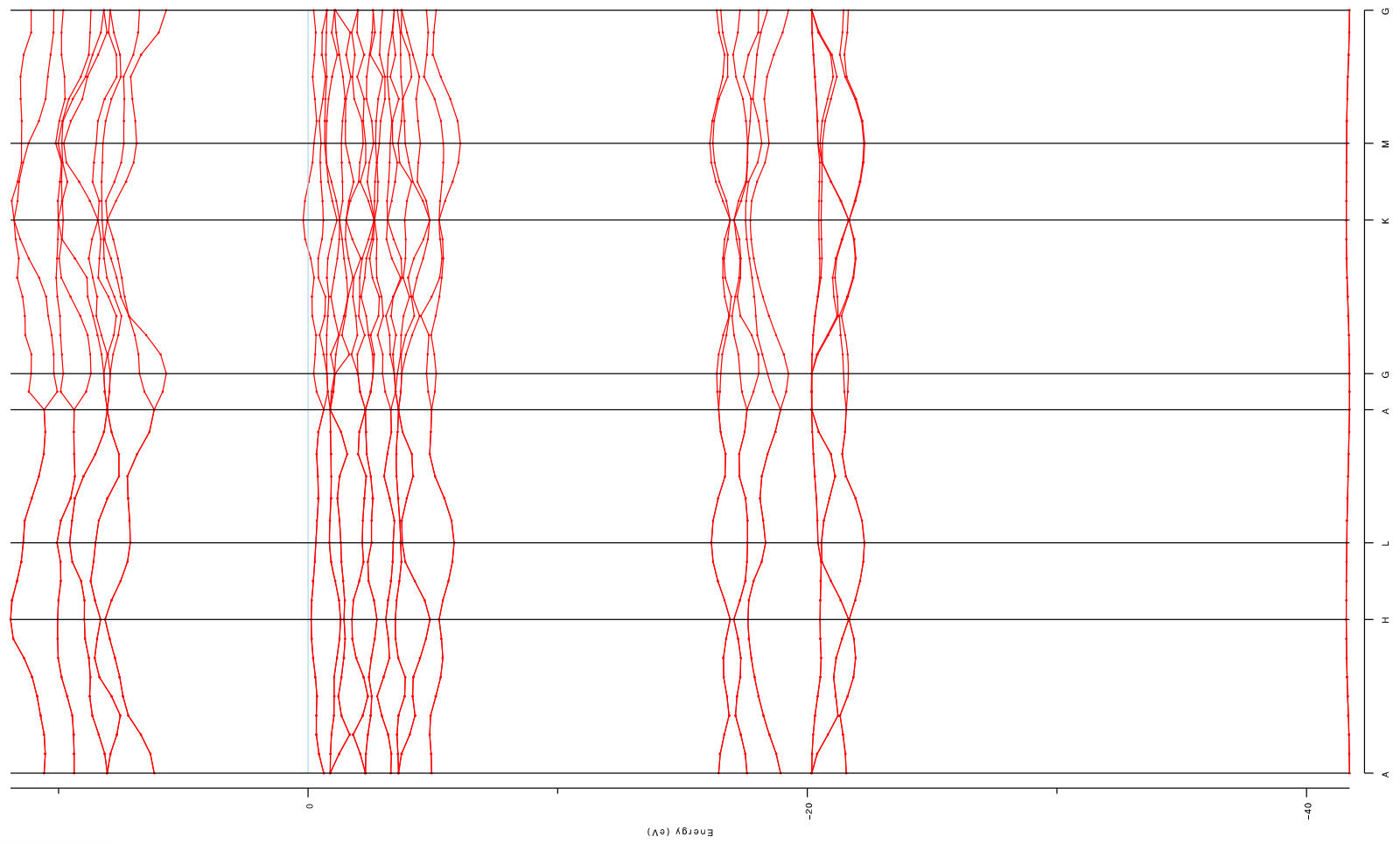
The phonon dispersions and density of states of the crystal of YCrO₃ and YCrO₄.

YAlO₃ (Pnma) Phonon

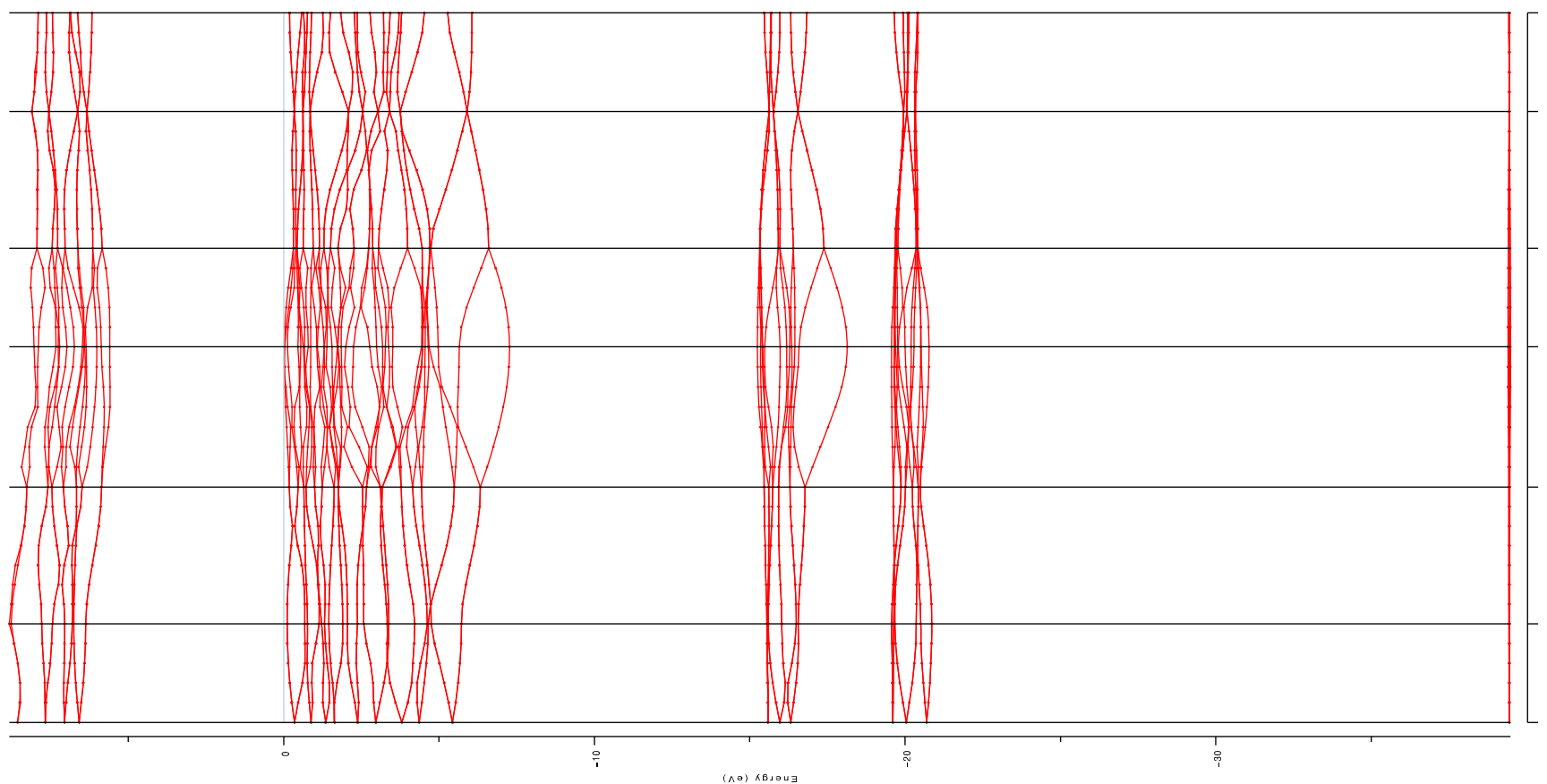
Phonon Dispersion for YAlO₃



YAlO₃ (P6_3mmc) GW Band Structure



YAlO₃ (Pnma) GW Band Structure



Publication and Awards

1. Papers published:

- “Nitrogen-doped fullerene as a potential catalyst for hydrogen fuel cells”, F. Gao, G. L. Zhao, S. Yang, and J. L. Spivey, *Journal of the American Chemical Society* **135**, 3315 (2013).
- “Catalytic reactions on the open-edge site of nitrogen-doped carbon nanotubes as cathode catalyst for hydrogen fuel cells”, F. Gao, G.L. Zhao, and S. Yang, *ACS Catalyst* **4**, 1267 (2014).
- “Detecting grain rotation at the nanoscale”, B. Chen, K. Lutker, J. Lei, J. Yan, S. Yang, and H.K. Mao, *PNAS* **111**, 3350 (2014).
- “Phase stability and hot corrosion behavior of ZrO_2 - Ta_2O_5 compound in Na_2SO_4 - V_2O_5 mixtures at elevated temperatures”, M. H. Habibi, S. Yang, and S. Guo, *Ceramic International* **40**, 4077 (2014).

2. Awards received:

- “Simulation and experiment study on high entropy alloy”, NASA/LaSPACE-LURA, with \$6,000, 1/1/2013 -- 12/31/2013.
- LINK award, NSF/LA-BOR, with \$6,000, 4/18/2014 – 6/30/2014.

Future Work

1. Continue to test the interface models and perform *ab initio* HPC simulation to study the stability, such as $\text{Y}_2\text{O}_3/\text{Fe}_3\text{Al}$ system based on the XRD data. The microstructures, elastic constants, and diffusion property will be simulated.
2. Experimentally validate the predicted ODS alloys: synthesize samples and characterize the high temperature and high pressure properties.
3. Students and postdocs training on ODS simulation and validation.

Acknowledgement

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- **Graduate students: Boliang Zhang, Lei Zhao, Jialin Lei, Cheng Guo, and Daniel Hart; undergraduate students: Michael Jackson, Megan Jones, and Yalin Liu.**
- **Postdocs: Drs. Liuxi Tan, Oleg Starovoytov.**
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Thank You

- Questions ?