

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

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Outline

Introduction
Methods
Preliminary Results
Future Work
Acknowledgement

Introduction

- Project Period: 6/1/2012 --- 5/31/2015
- Project Manager: 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 Preliminary Results

1. 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 (P6₃mmc and Pnma) this is 5.91 eV and 6.62 eV, which are insulators.

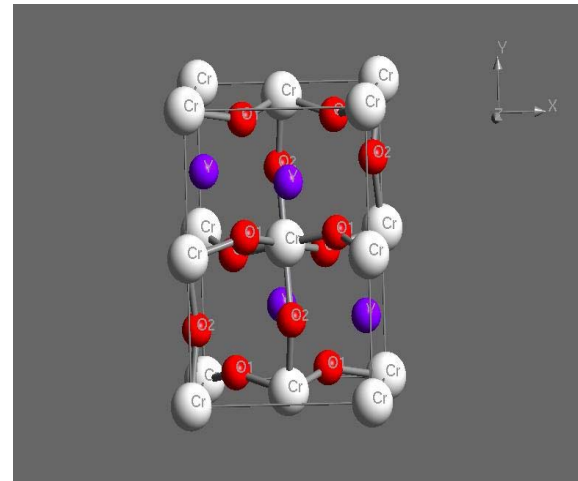
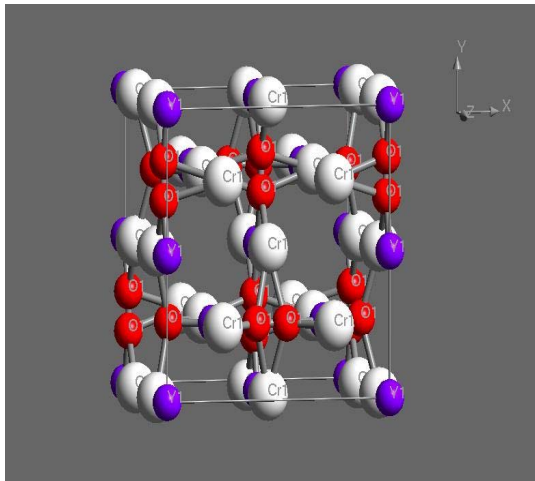
The phonon calculations show that the main difference between YCrO_3 supercell and YCrO_4 supercell phonon dispersion curves is in YCrO_3 supercell phonon dispersion curve, there is an extra high frequency phonon band from 25 THz ~ 28 THz while in YCrO_3 supercell curve the phonon is continuous from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

Current Status and Achievements

2. The MA956 samples with 20% Cr 4.5 % Al, 0.5 Ti, 0.5% Y_2O_3 and balance Fe were tested and the data is processing. The test results will provide info for a good Fe/YTiCrO simulation models.

As a model high pressure experimental system, the NiS sample was tested with high pressure radial synchrotron XRD. The NiS results show that the S concentration increase from 7% to 20% makes the NiS brittle.

YCrO_3 and YCrO_4 Simulation



YCrO_4 and YCrO_3 structures used in our simulation. Both have rectangular structures. The blue balls stand for Y atoms, white balls for Cr atoms while red balls for O atoms.

YCrO₃ Elastic Constants

Modulus	Voigt	Reuss	Hill

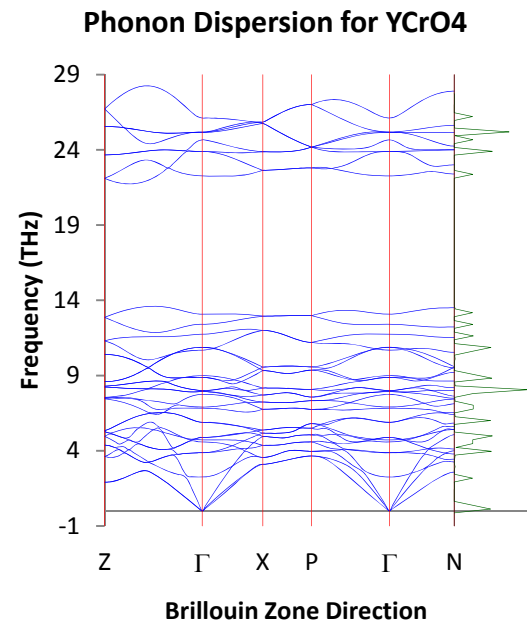
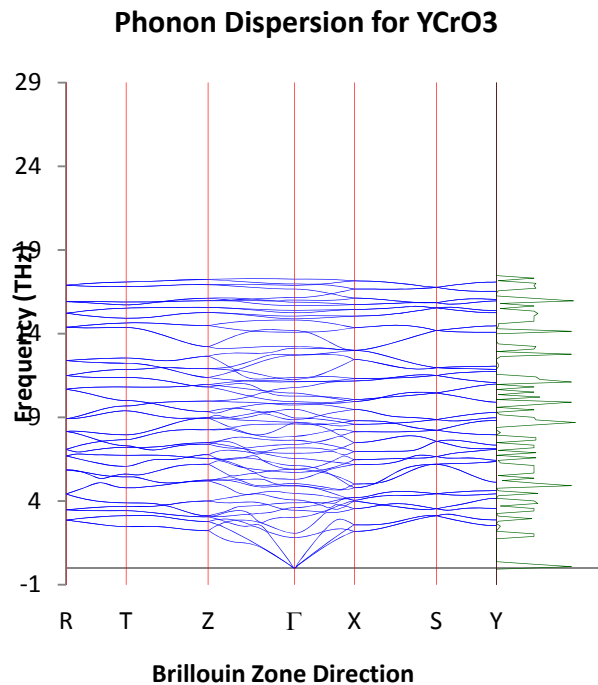
Bulk	189.91	189.52	189.72 GPa
Shear	99.13	95.25	97.19
Young's	253.31	244.75	249.03
Longitudinal			319.30

Velocity of sound

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

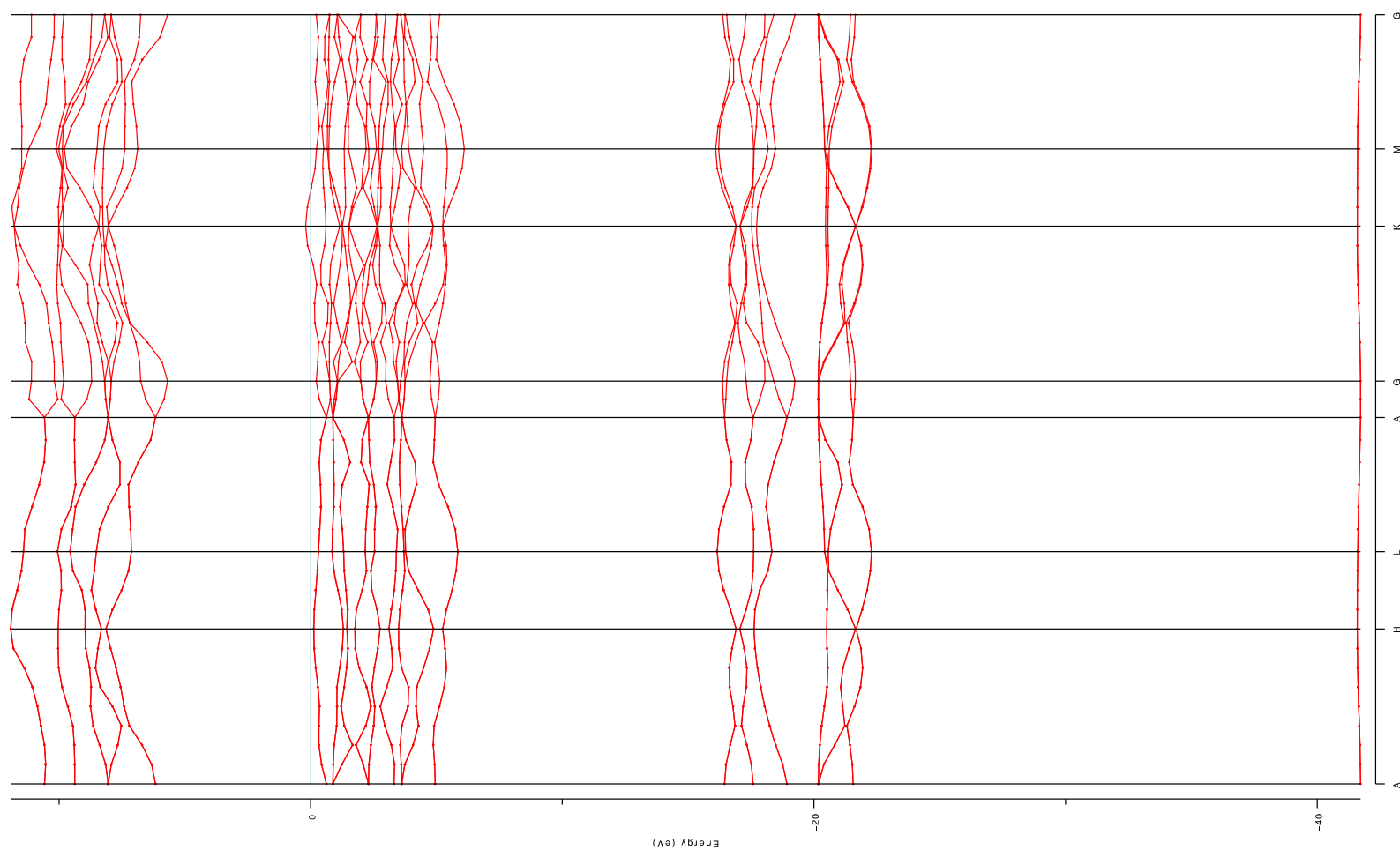
Debye temperature: 608.0 K

YCrO₃ and YCrO₄ Phonon Dispersion and DOS

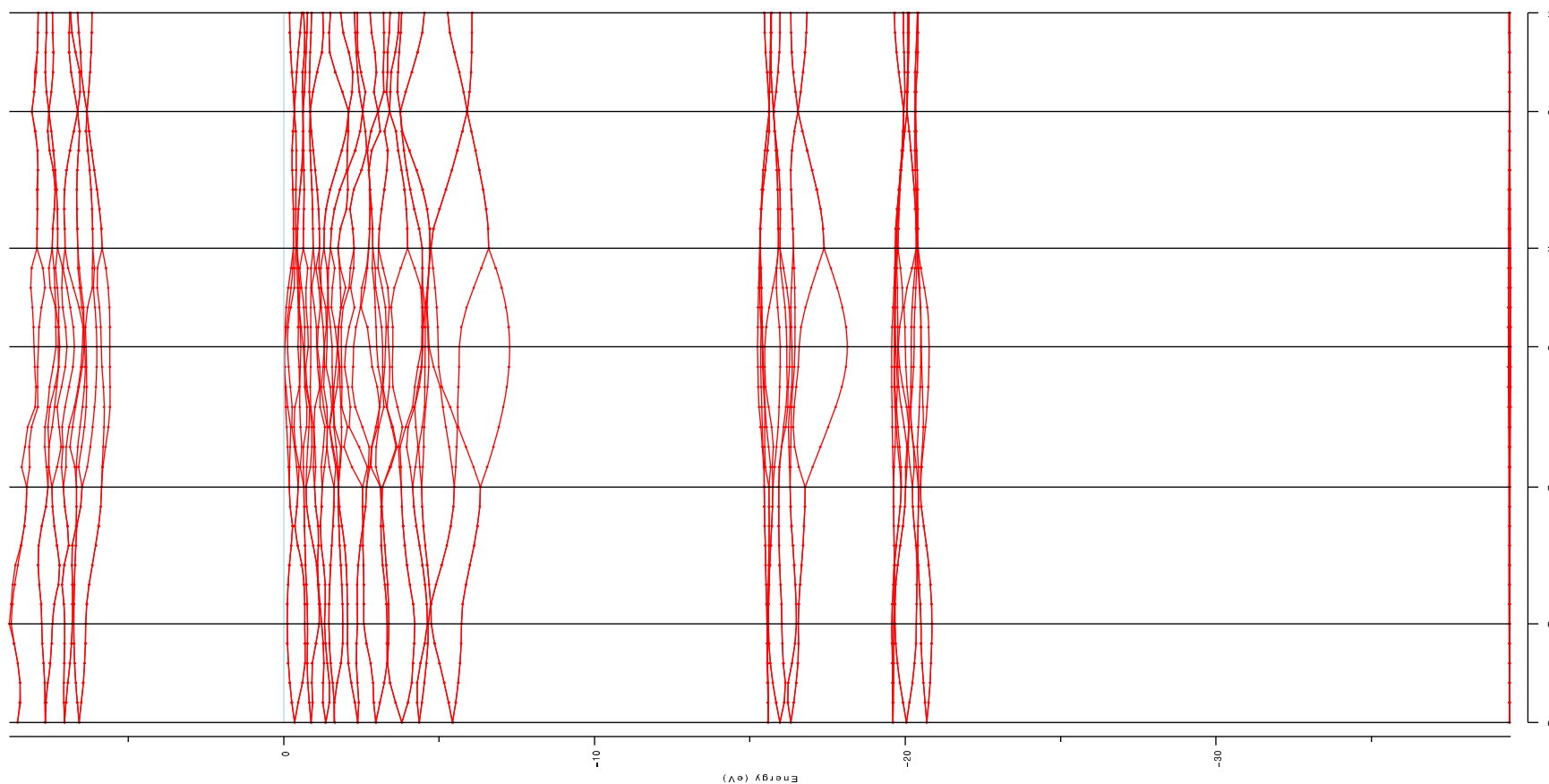


The phonon dispersions and density of states of the crystal of YCrO₃ and YCrO₄.

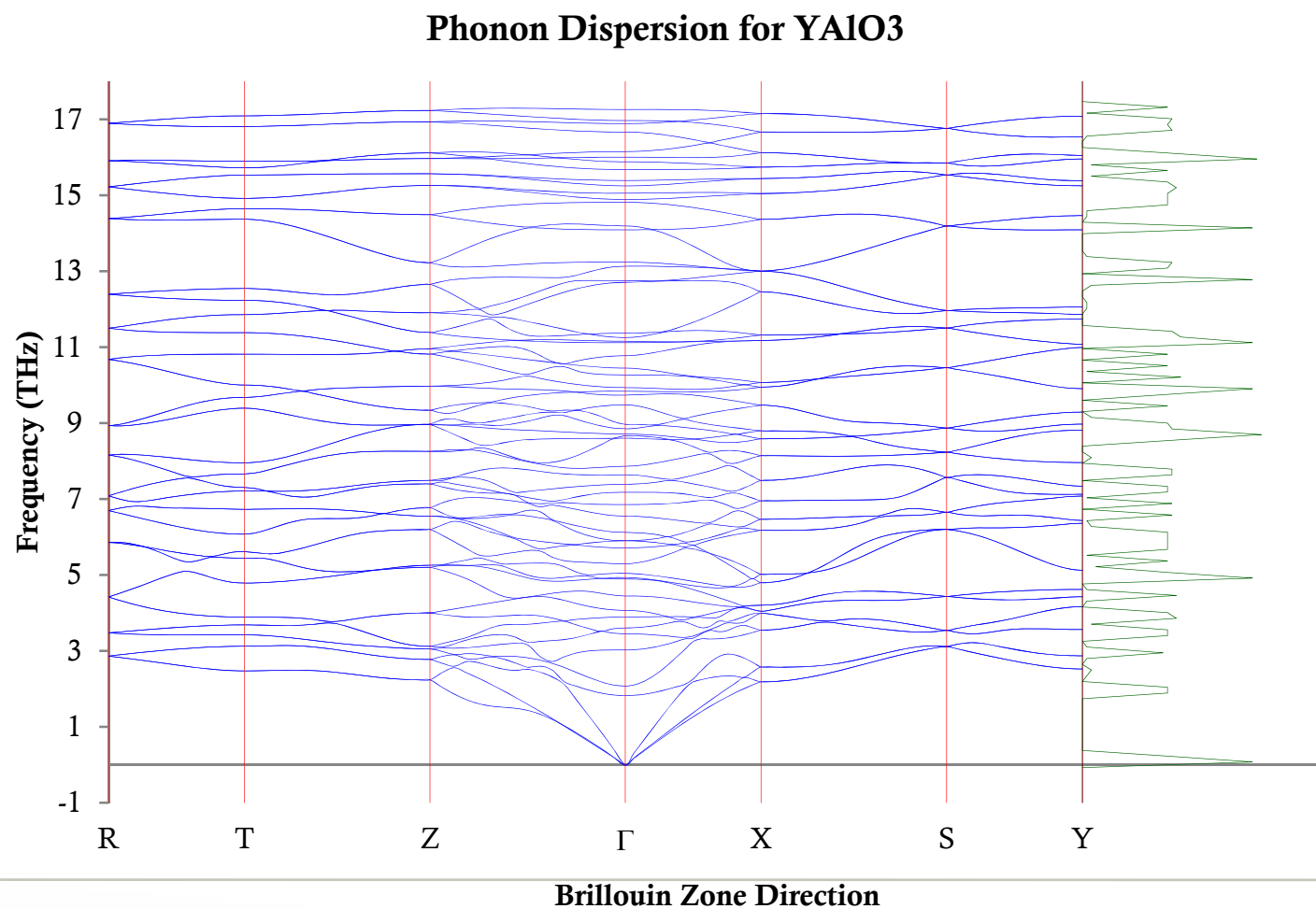
YAlO₃ (P6₃mmc) GW Band Structure



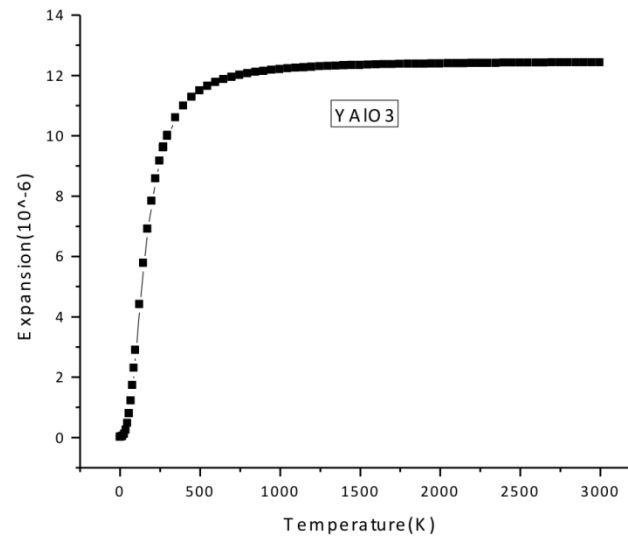
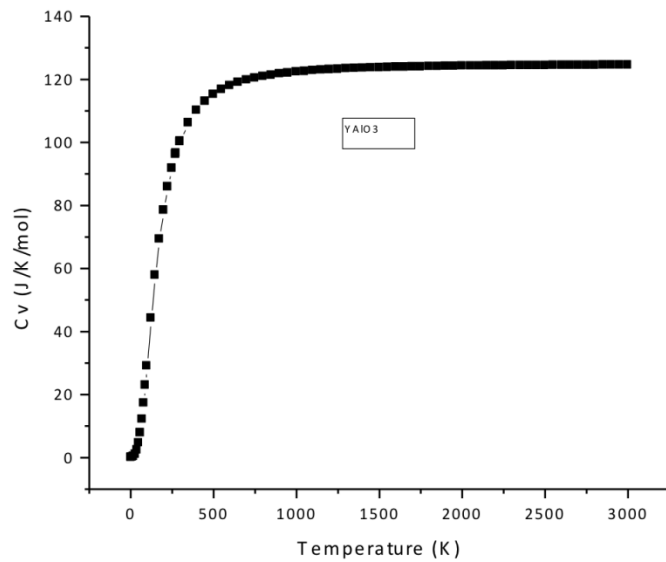
YAlO₃ (Pnma) GW Band Structure



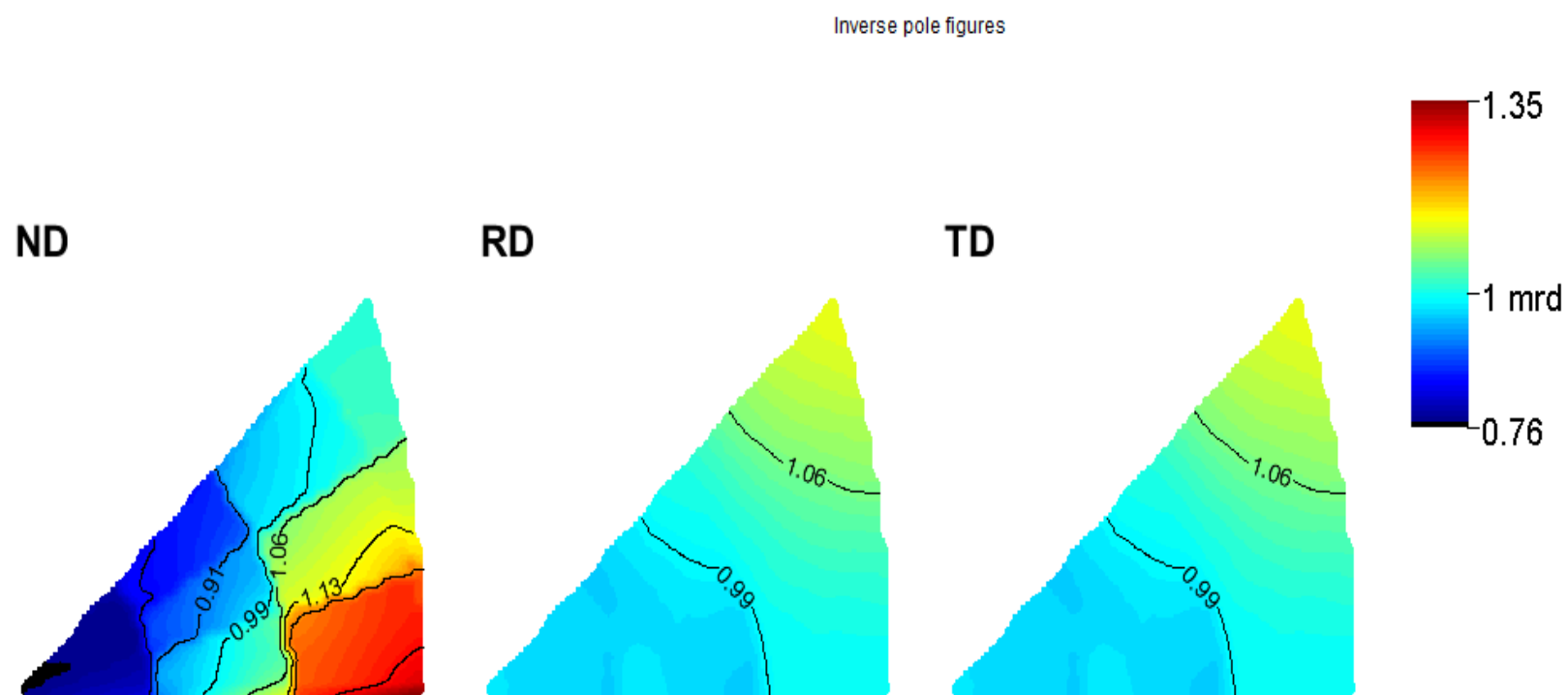
YAlO₃ (Pnma) Phonon



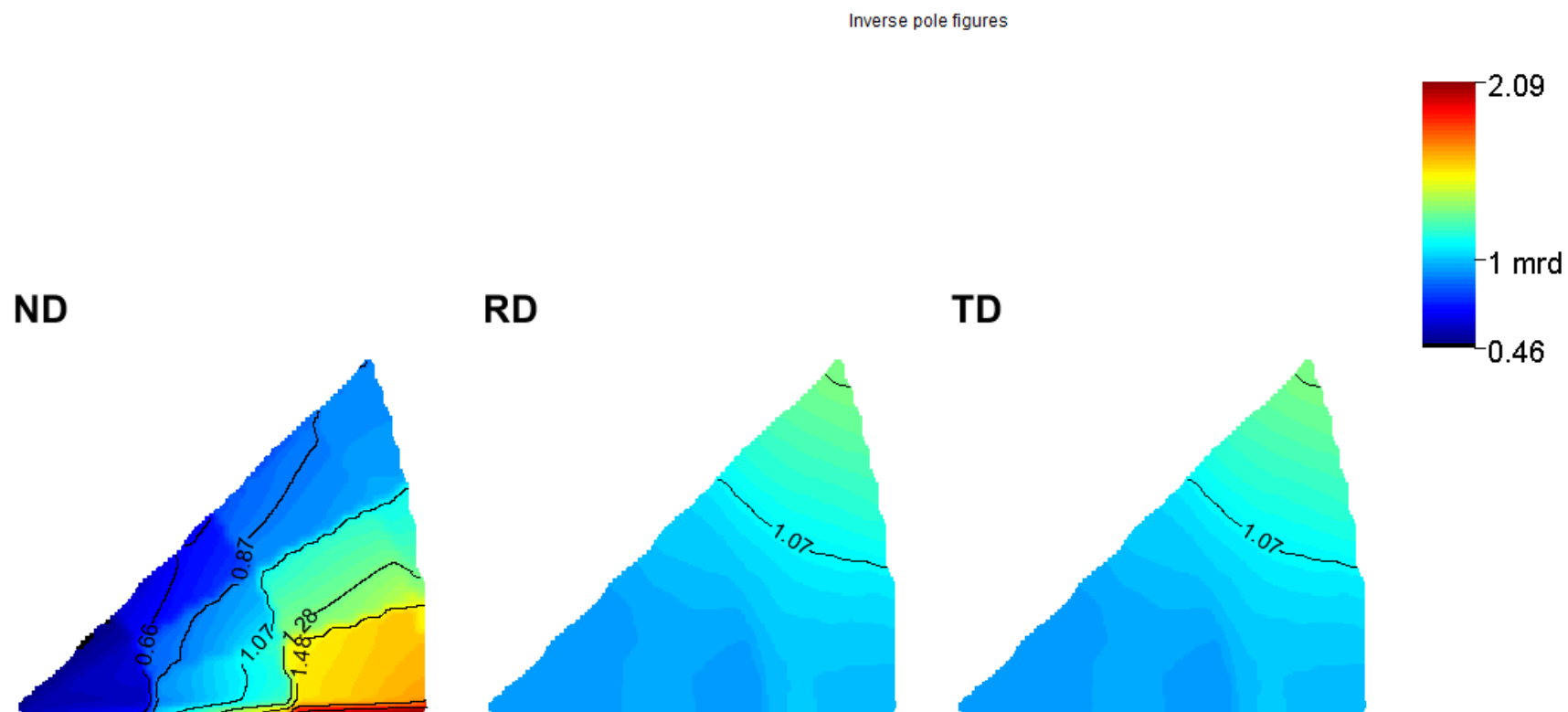
Heat Capacity and Thermal Expansion of YAlO_3



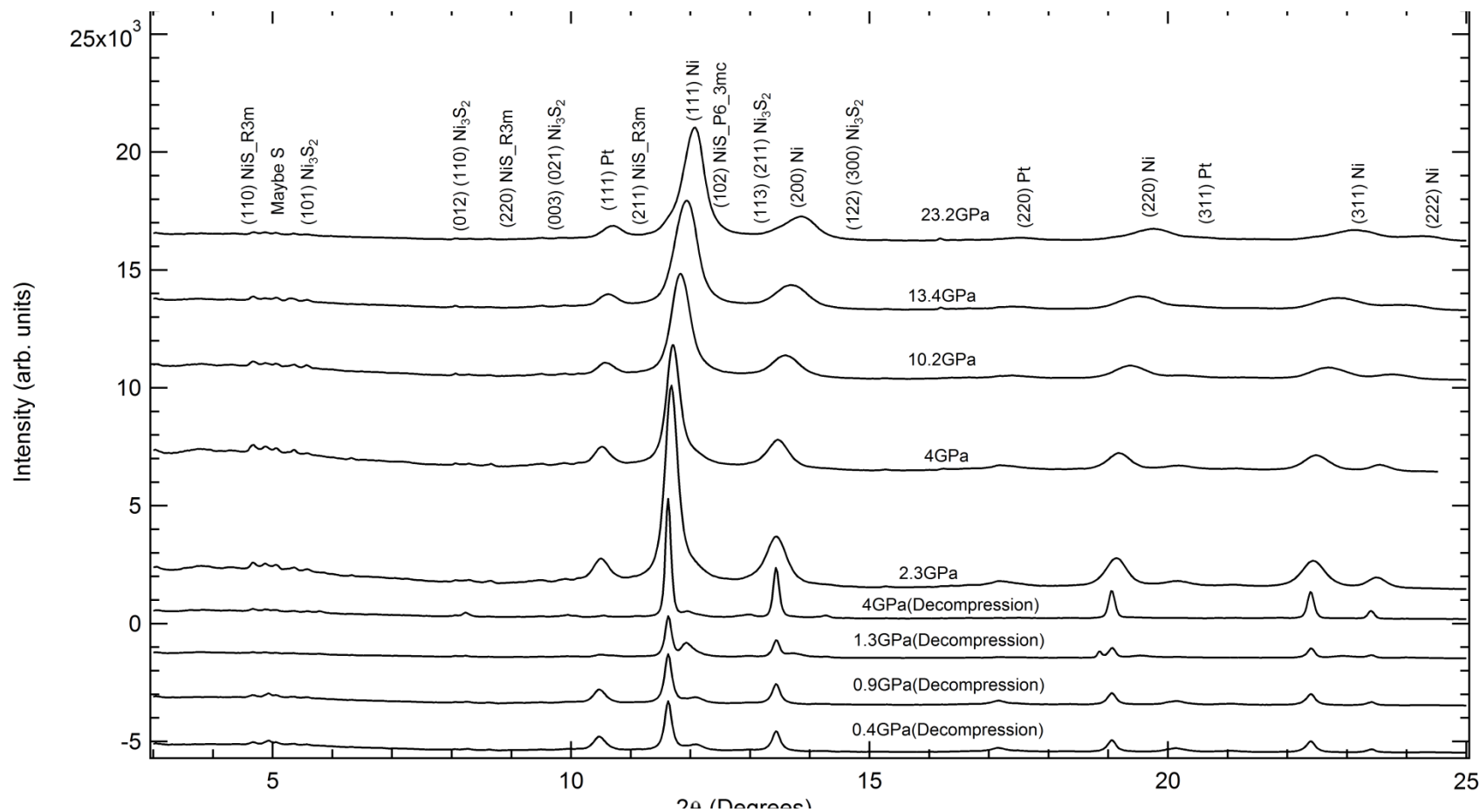
S doped 7% NiS 4.5 GPa Texture



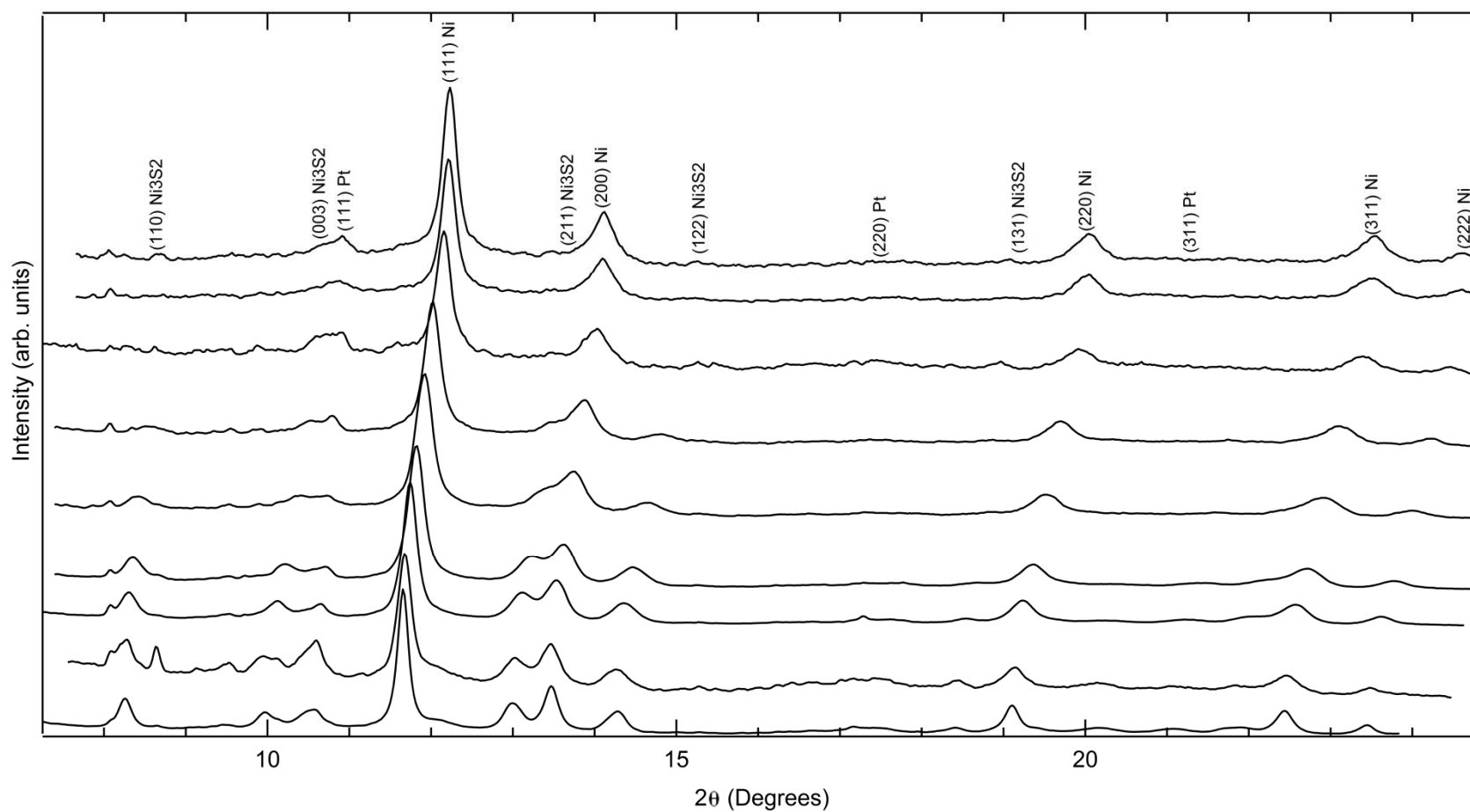
S doped 7% NiS 9.6 GPa Texture



S doped 7% NiS Synchrotron Radial XRD



S doped 20% NiS Synchrotron Radial XRD



Summary

1. The interface compounds YCrO_4 , YCrO_3 , and YAlO_3 were simulated by *ab initio* density functional theory method.
2. 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 (P6₃mmc and Pnma) this is 5.91 eV and 6.62 eV, which are insulators.
3. The sample ODS was tested. As a model high pressure experimental system, the S doped NiS samples were tested with high pressure radial synchrotron XRD. The NiS results show that the S concentration increase from 7% to 20% makes the NiS brittle and along with Ni_3S_2 phase transition.

Publication and Presentations

1. Paper 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).

2. Conference presentations:

- “Oxygen molecule adsorption and dissociation on boron-doped fullerene BC_{59} ” Shizhong Yang, Lei Zhao, Feng Gao, Guang-Lin Zhao, Ebrahim Khosravi, and Diola Bagayoko, APS March Meeting, Baltimore, Maryland, March 2013.
- “Comparative studies of the ground state properties for $Nb_{25}Mo_{25}Ta_{25}W_{25}$ and $V_{20}Nb_{20}Mo_{20}Ta_{20}W_{20}$ alloys”, Oleg N. Starovoytov, Michael Gao, Shengmin Guo, Ebrahim Khosravi, Jialin Lei, Liuxi Tan, and Shizhong Yang, TMS 2013 Annual Meeting, San Antonio, Texas, March 2013.
- “Oxidation behavior of TaNbHfZrTi alloy: a first principles simulation study”, Shizhong Yang, Michael Gao, and Shengmin Guo, TMS 2013 Annual Meeting, San Antonio, Texas, March 2013.

Presentations/Awards

- “Properties of zirconia gadolinia ytterbia yttria thermal barrier coating studied by first principles simulation”, Liuxi Tan, Lei Zhao, Shengmin Guo, Ebrahim Khosravi, and Shizhong Yang, TMS 2013 Annual Meeting, San Antonio, Texas, March 2013.
- “Research projects of HPC Group at Southern University”, Shizhong Yang, Liuxi Tan, Jialin Lei, Cheng Guo, Michael Jackson, Shengmin Guo, and Ebrahim Khosravi, Invited Talk at LONI HPC User Symposium, Baton Rouge, Louisiana, June 2013.

3. Awards received:

- “Simulation and experiment study on high entropy alloy”, NASA/LaSPACE-LURA, with \$6,000, 1/1/2013 -- 12/31/2013.

Future Work

1. Continue to test the interface models and perform *ab initio* HPC simulation to study the stability. 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

- Graduate students: Lei Zhao, Jialin Lei, Cheng Guo; undergraduate students: Michael Jackson and Yalin Liu.
- Postdocs: Drs. Liuxi Tan, Oleg Starovoytov.
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