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

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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 validation on the high temperature and high pressure property of the most promising ODS systems from the simulation.

(3). Students/postdocs training on material simulation and experiment validation: synthesis, XRD, TGA, DSC, synchrotron XRD texture.

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 (Y) and Chromium (Cr)) 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.

Introduction

Recent advance on Y doping in ODS research:

- The Y_2O_3 -TiO_2 nanometer complex oxide increases the ODS creep and rupture strength greatly.
- The Y_2O_3/ (Cu, Al) ODS were investigated at 1423 K and the $YAlO_3$ formed.
- The implanted compounds change from Y_2O_3 to $Y_3Fe_5O_{12}$ and $YFeO_3$ when the temperature increases from 200℃ to 570℃.
- In-situ high temperature (700℃) oxidized pure iron with Y implanted shows the oxidation compounds Fe_2O_3, Fe_3O_4, $YFeO_3$ and YFe_2O_4 after high temperature oxidation.

see e.g.: Prog. Nat. Sci.: Mat. Int. 23, 434 (2013)

Mat. Chem. Phys. 64, 29 (2000)

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.

Results and Current Status

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

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 $YCrO_4$ 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.

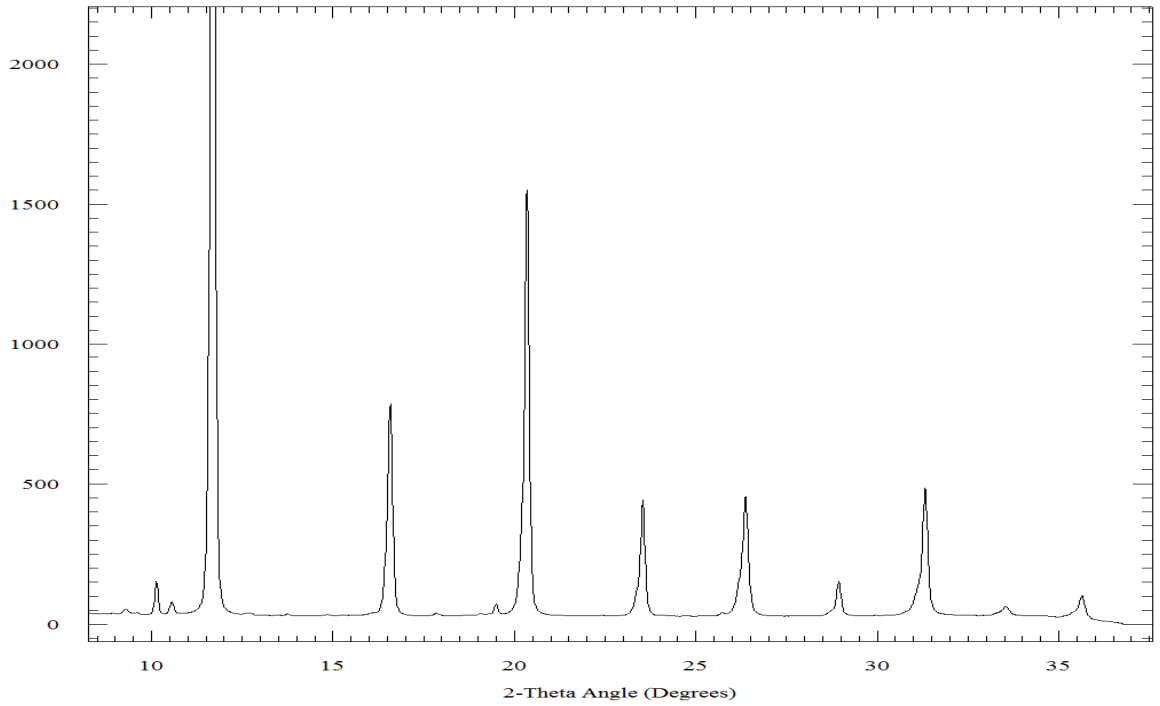
Results and Current Status

2. 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.

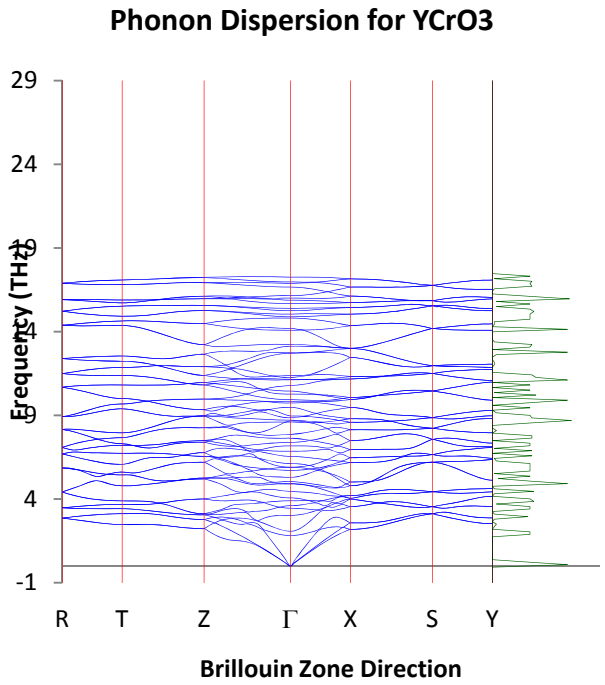
The test results provides info for a good Fe/YTiCrAlO simulation models.

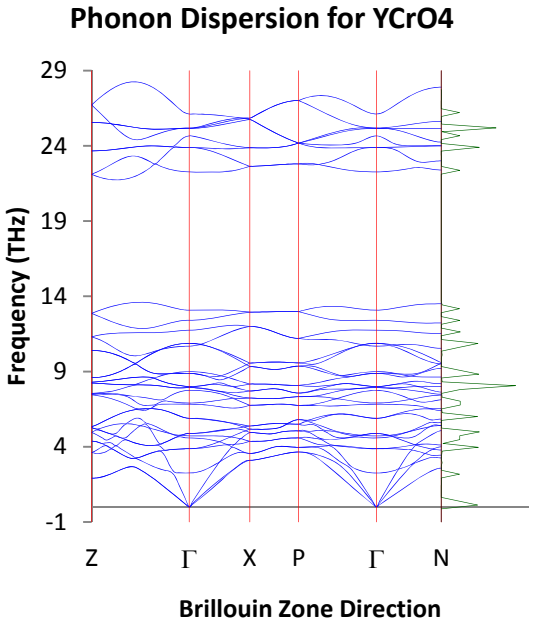
The Ambient Pressure XRD Results



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

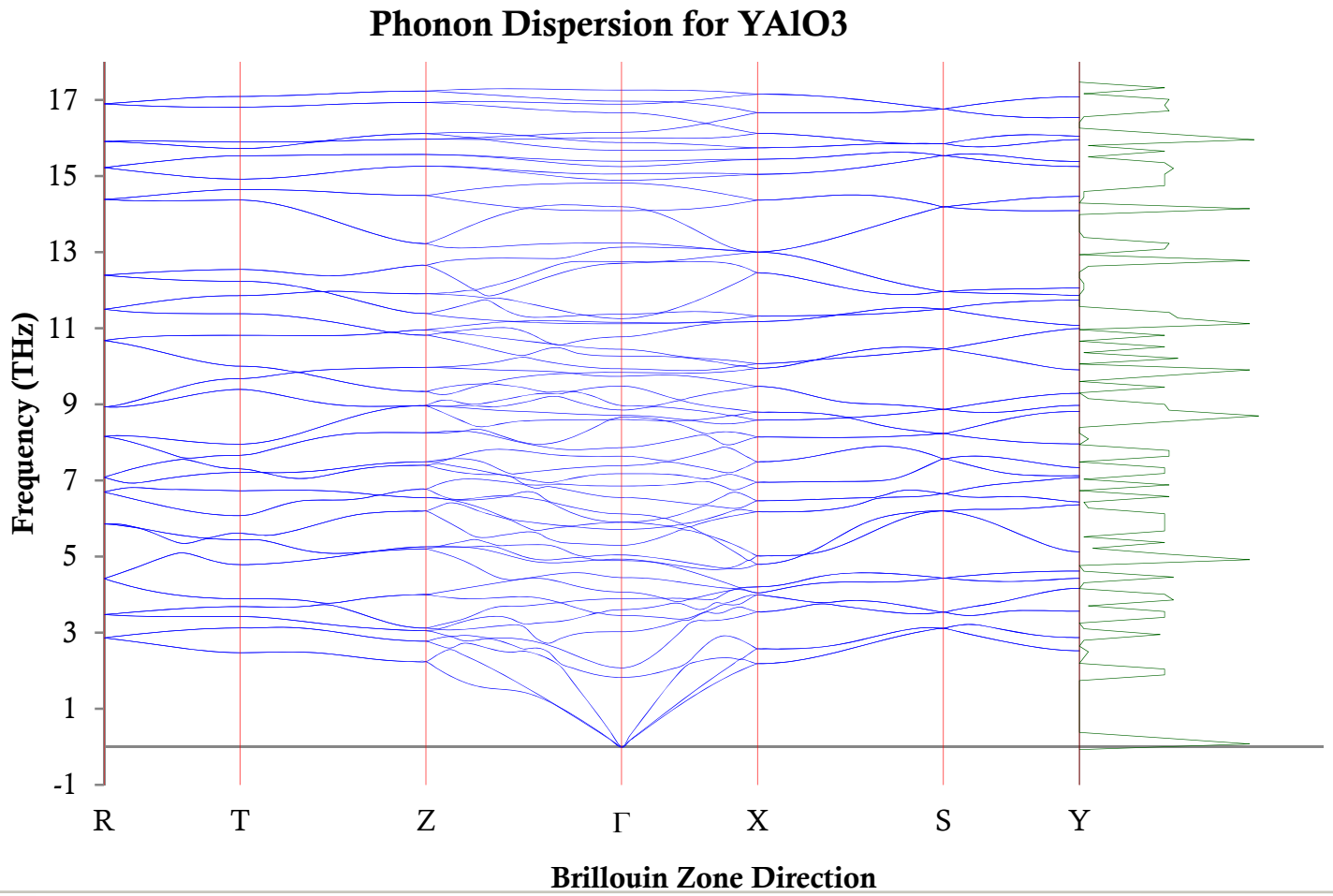
$YCrO_3$ and YCrO4 Phonon and DOS





The phonon dispersions and density of states of the crystal of $YCrO_3$ and $YCrO_4$.

$YAlO_3$ (Pnma) Phonon and DOS

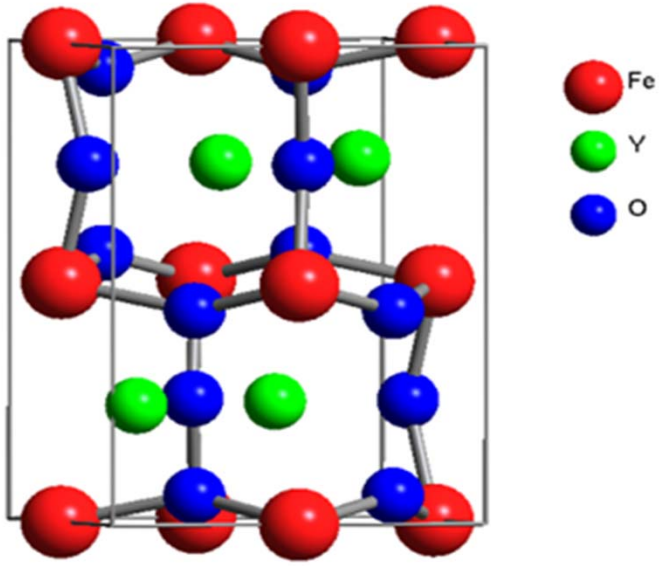


Results and Current Status

3. Electronic Structure and Mechanical Property of $YFeO_3$ under Pressure: Recent research indicates $YFeO_3$ may improve the oxidation resistance at high temperature. The properties of $YFeO_3$ are investigated by DFT based first principles simulation, sample synthesis and characterization, and synchrotron XRD texture measurement under high pressure shear stress.

$YFeO_3$ Model Simulation

- VASP-the first principles density functional theory.
- The $YFeO_3$ crystal model includes 4 Fe atoms, 4 Y atoms and 12 O atoms within a 5.4 Å × 7.2 Å × 5.0 Å cell.



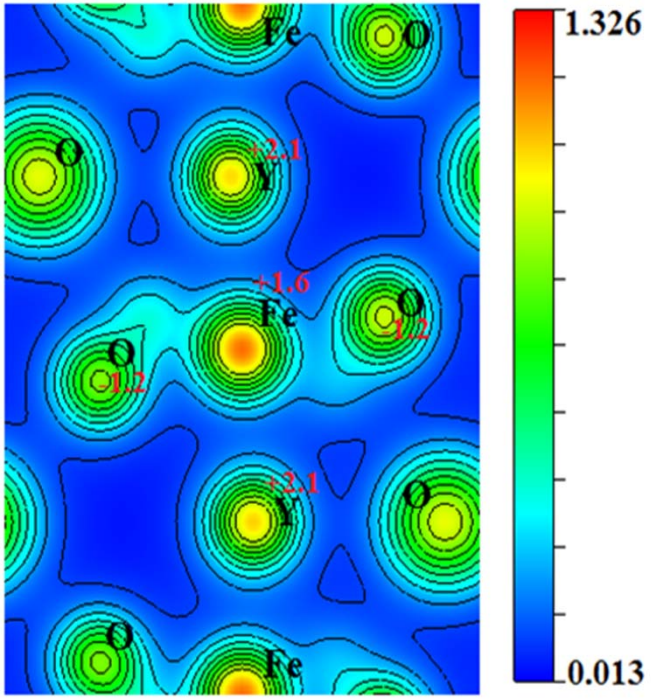
Elastic Matrix of YFeO3

C_{ij} (GPa)	1	2	3	4	5	6
1	357.70	212.85	220.30	0	0	0
2	212.85	399.80	175.95	0	0	0
3	220.30	175.95	359.3	0	0	0
4	0	0	0	84.20	0	0
5	0	0	0	0	106.80	0
6	0	0	0	0	0	133.20

C44 > 0, C11 > |C12|, and C11+2C12 > 0.

2D Charge Density

- The (001) plane .
- Each Y (+2.1 |e|) lose more than two electrons.
- For Fe, the electrons in both 3d and 4s orbitals are activated because each Fe (+1.6 |e|) lose more than one electron.
- For O, the 2p orbital has 4 electrons and can act as electron acceptor. So each O (-1.2 |e|) get more than one electron.

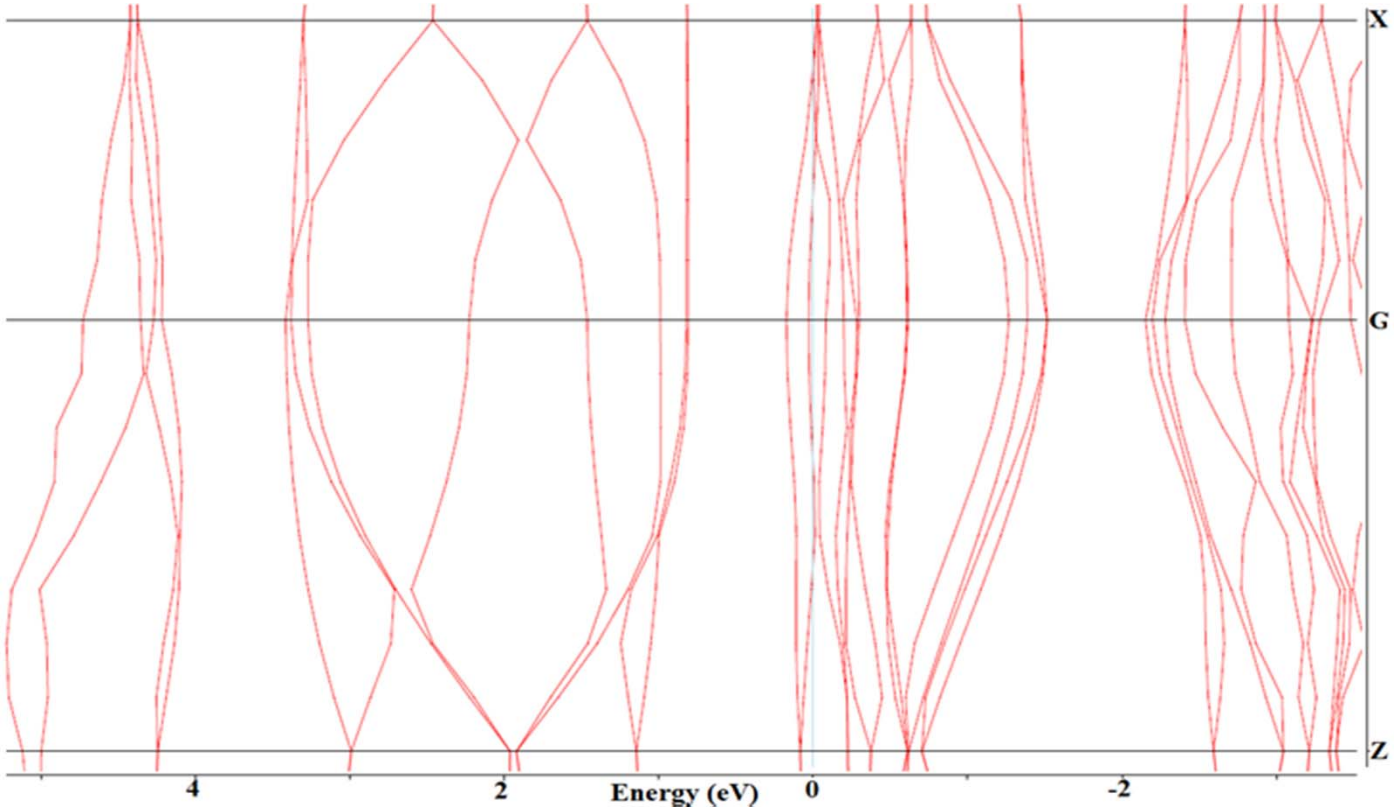


Electrons and Distance Change under Pressure

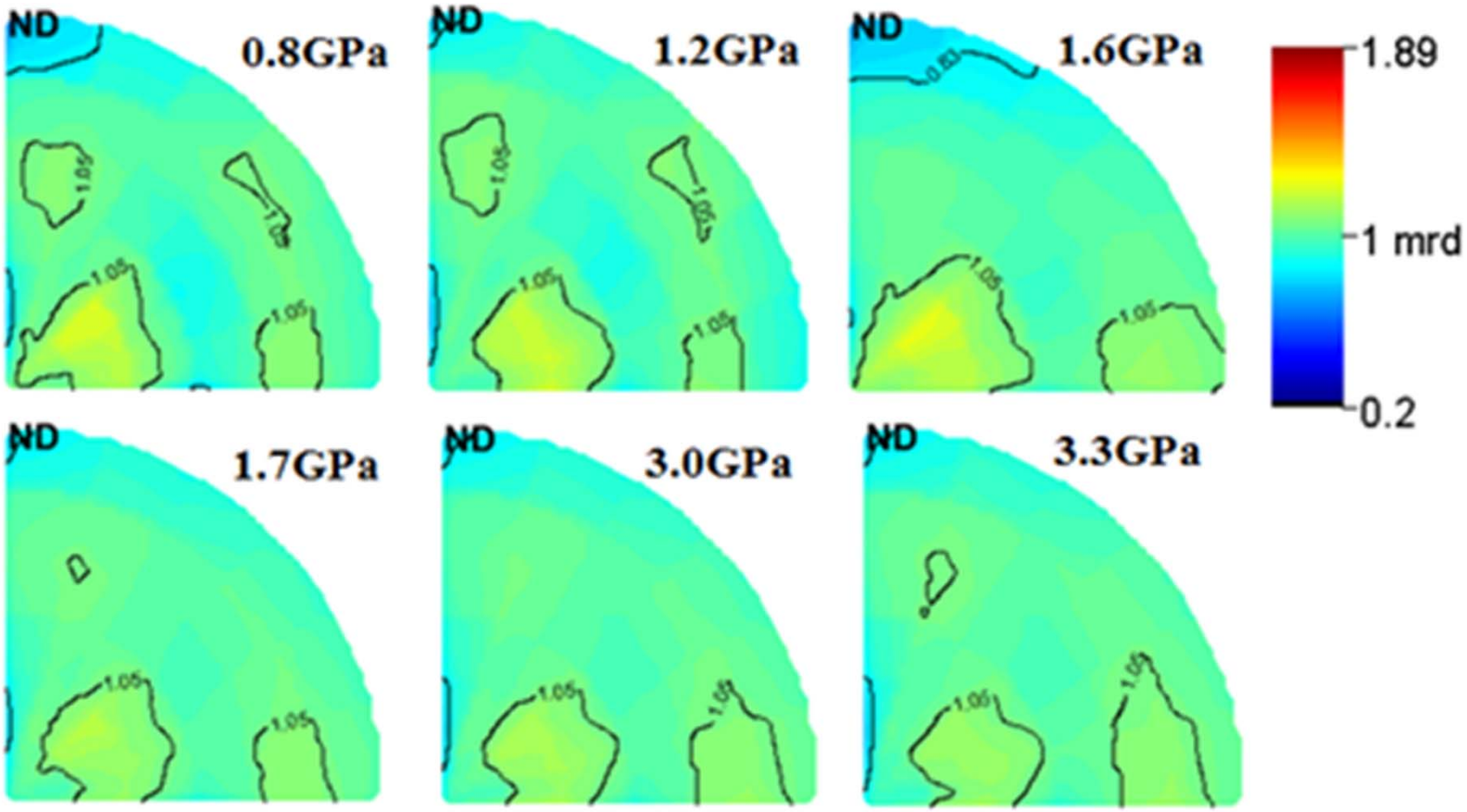
- The lost and gain of electrons are balanced.
- When the compact pressure increases from 3.3 GPa to 90 Gpa, the minimum distances between Fe and O change from 1.86 Å to 1.84 Å (small) and the minimum distances between Y and O change from 2.62 Å to 2.15 Å (large). i.e. Fe-O is very stable while Y-O adjust to the external pressure changes.

Band Structure

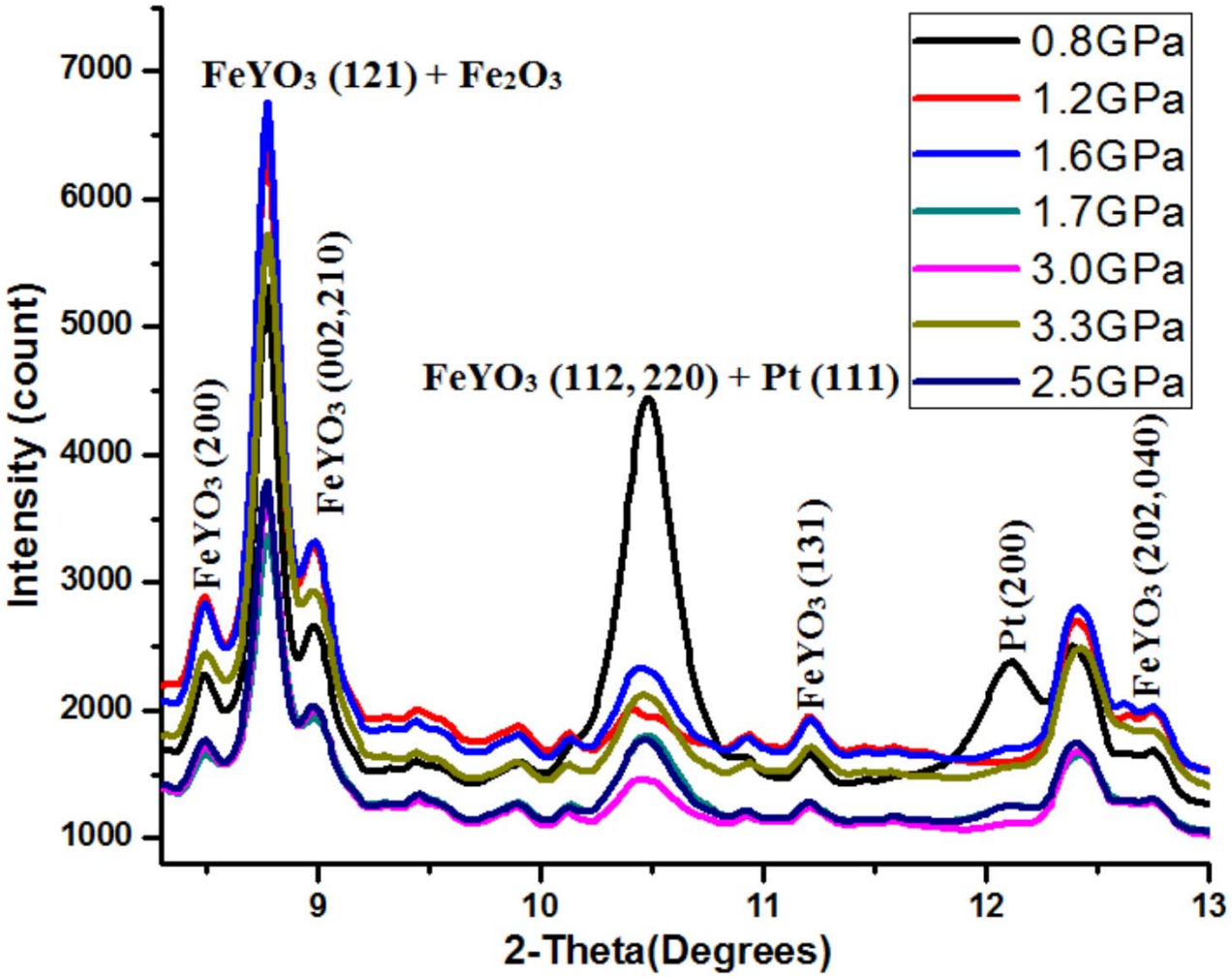
- The direct band gap is 0.64 eV. (semiconductor)



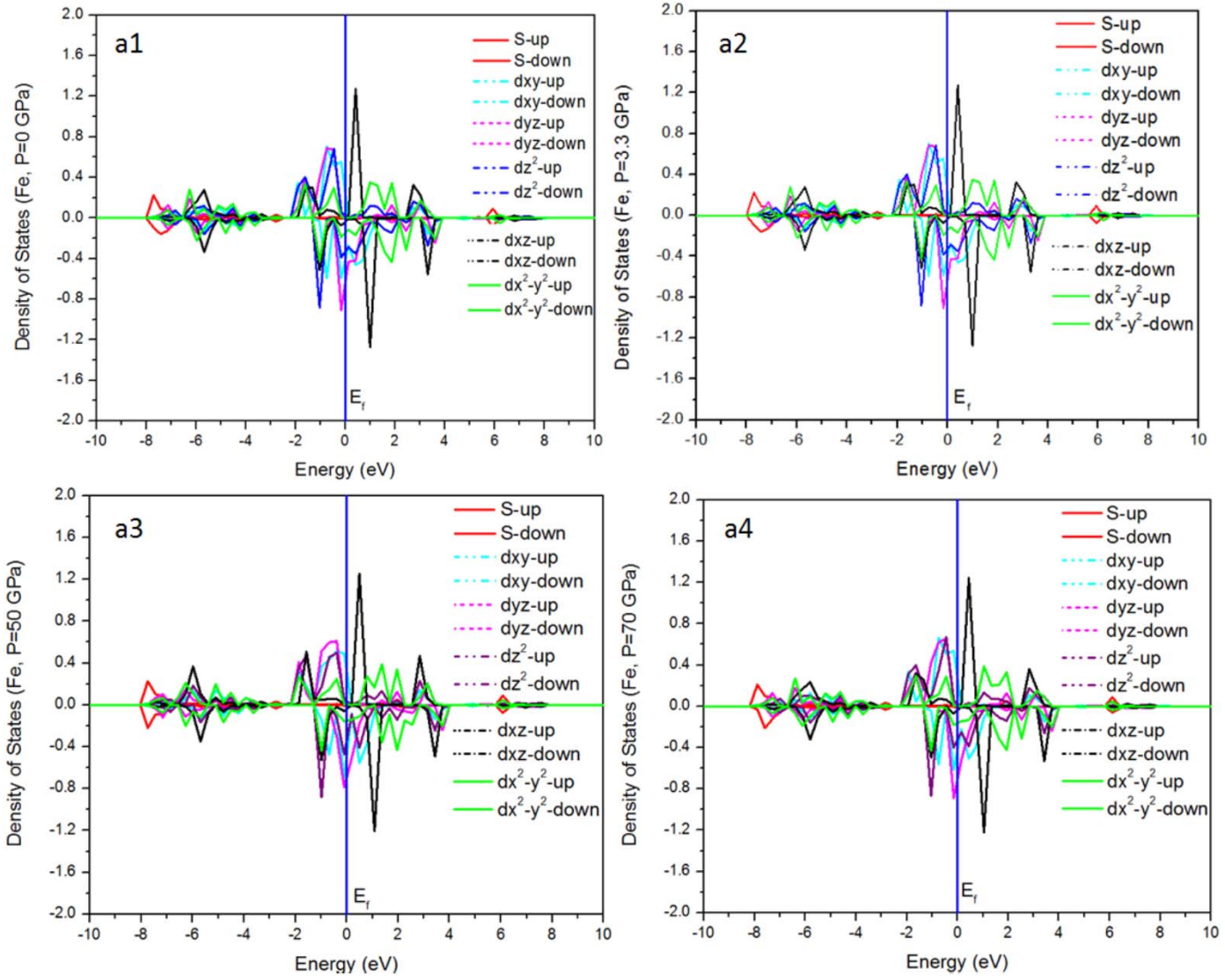
Texture Analysis



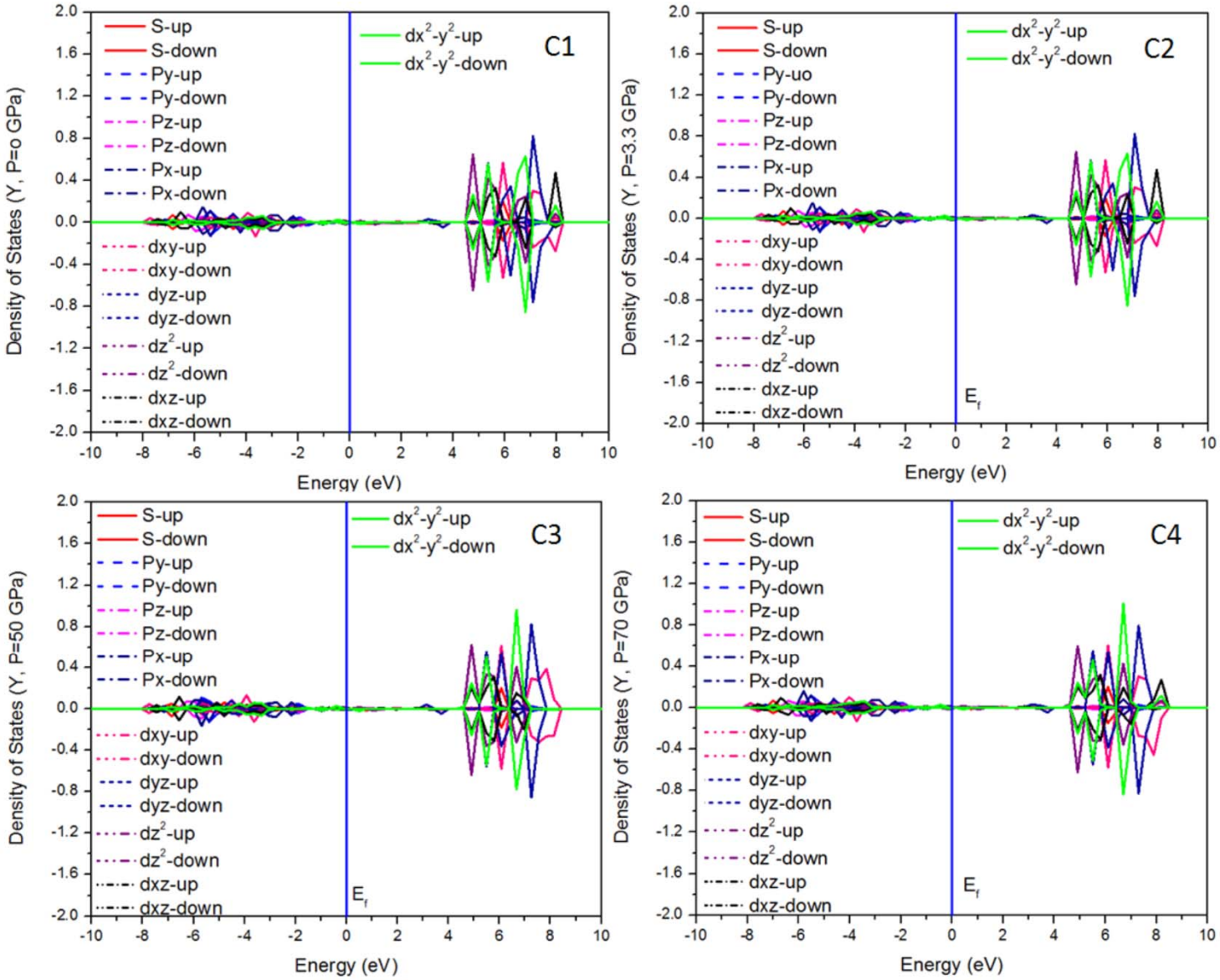
XRD under Compression Pressure



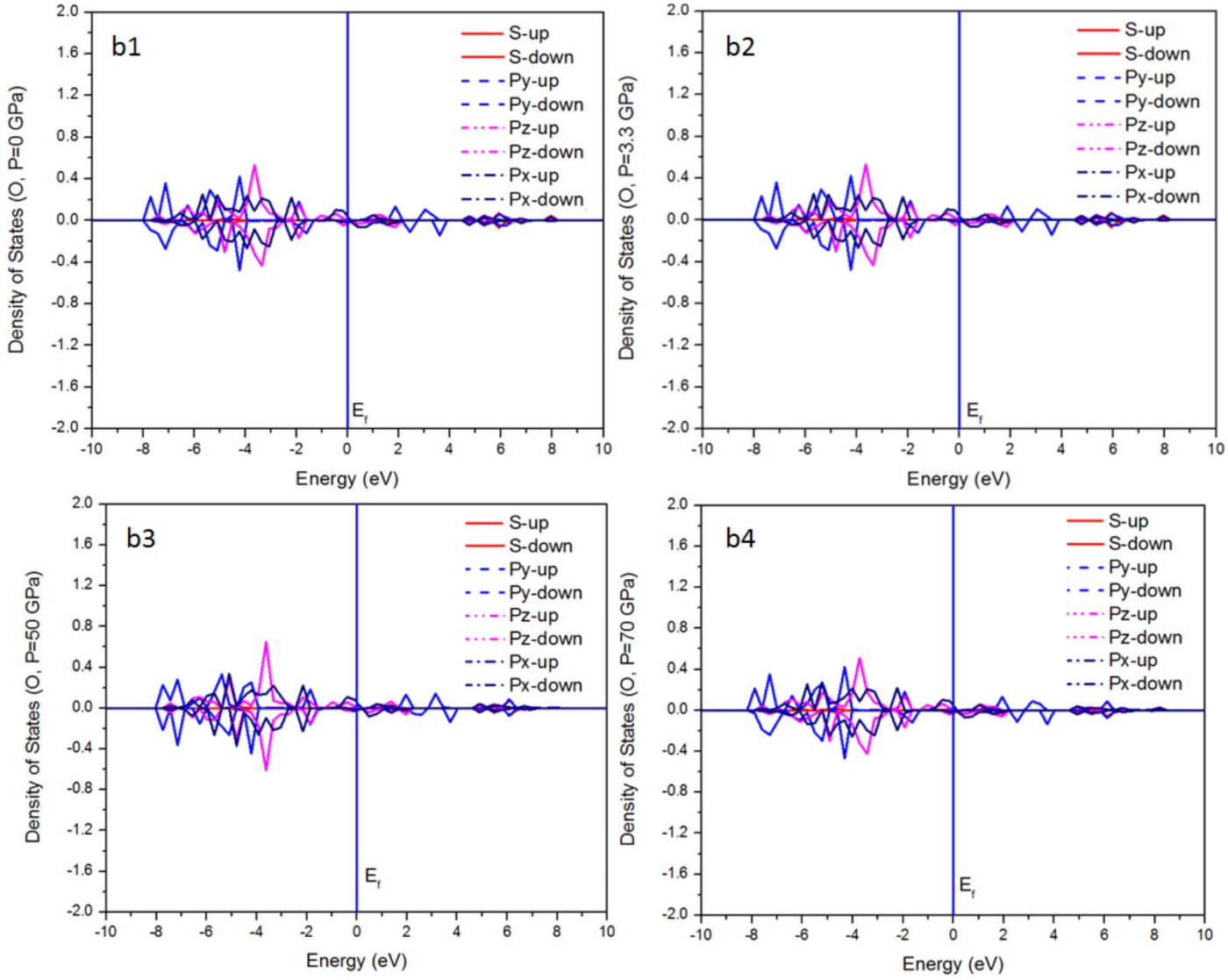
Density of States Analysis -Fe



Density of States Analysis -Y



Density of States Analysis -O



Summary on $YFeO_3$ Study

- The $YFeO_3$ have stable mechanical properties until up to 3.3 Gpa.
- From DFT simulation simulation the electronic and mechanical properties are stable up to 90 Gpa.
- The relative stable properties is from the Fe-O stable bonding and Y-O flexible adjustment.
- The texture study shows dislocation pinning effect in $FeYO_3$ under 3.3 Gpa.

Publication and Awards

1. Papers published:

- "Senary refractory high entry alloy MoNbTaTiVW", B. Zhang, M. Gao, Y. Zhang, S. Yang, and S. Guo, Materials Science and Technology, 2015, in printing.
- "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).
- "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).

Awards

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 – 4/17/2014.
- RAP Award, "Materials Design and Process Optimization for Selective Laser Melting Based Advanced Manufacturing", LASPACE, $89,851, 12/1/2014 – 10/31/2015 (PI: Guo, Co-PI: Yang).

Future Work

1. Continue to test the interface models and perform *ab initio* DFT HPC simulation to screen the optimized candidates. The 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, Yan Yang, and Xiaoping Wang; undergraduate students: Michael Jackson and Yalin Liu.
- Postdocs: Drs. Liuxi Tan, Oleg Starovoytov.
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