Molecular Dynamics Simulation and Experimental Validation on Cr-based Alloys

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5/31/2012 Pittsburgh, PA

Outline

Introduction
Method
Cr-Y Alloy Simulation and Experiment
Future Work
Acknowledgement

Introduction

- Project Period: 10/1/2010 --- 12/31/2012
- Project Manager: Steve Markovich
- Project Objectives:

  (1). Building reliable *ab initio* interatomic potentials.

  (2). Perform HPC simulation on the model systems.

  (3). Perform experimental validation.

Introduction

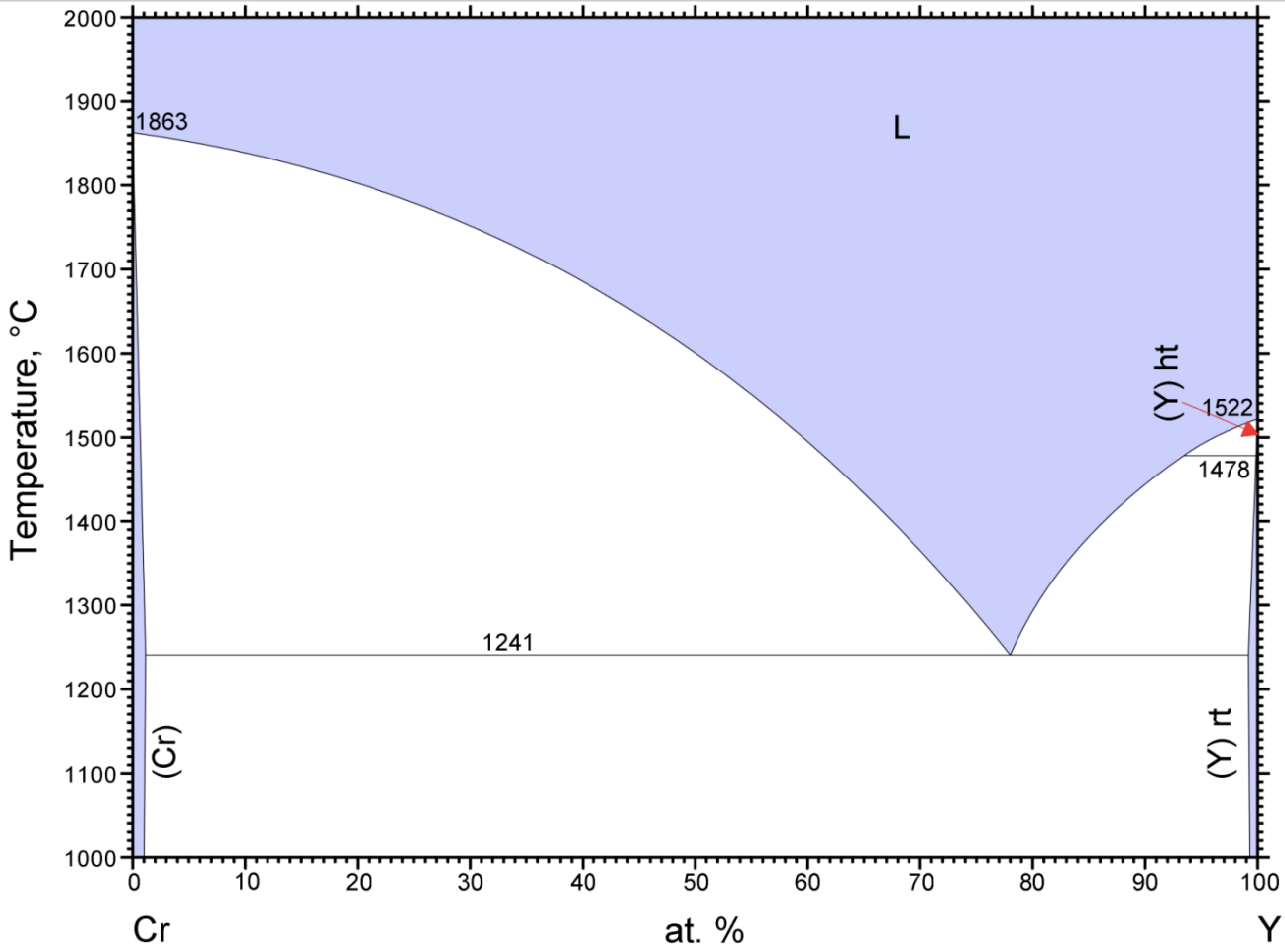
Cr-based alloys have advantages:

high melting point (Cr 1907°C), low cost, low density, and high temperature strength.

Disadvantages: high T oxidation and low T ductility.

Benefits of Cr based alloys: The doping of transition metals such as Y, Ce and La in Cr-based alloys can reduce the residual oxygen content in the bulk by forming very stable oxides to enhance extrinsic ductility. The slow diffusivities of these dopants and dispersion strengthened oxides increase the creep resistance of Cr-based alloys.

Cr-Y Phase Diagram



Current Available Methods

- **Current *ab initio* MD method is accurate but is time consuming and expensive for large systems like >500 atoms.**
- **Classical MD on the other hand is fast and efficient but the accuracy of the results is depending on the accuracy of the potentials used in the simulation.**
- **We are integrating both the current *ab initio* and classical MD methods to facilitate simulations.**

Method We Used

- **Ab initio potential generating code test.**

$$E_{total}(\rho) = T + \sum_{lm}\int \rho(\vec{r})dv\frac{-e^2 Z_m}{\left|\vec{r}-\vec{\tau}_m-\vec{R}_l\right|}+\frac{1}{2}\int\frac{\rho(\vec{r})\rho(\vec{r}')}{\left|\vec{r}-\vec{r}'\right|}dvdv'+E_{xc}(\rho)+\frac{1}{2}\sum_{mn}\frac{e^2 Z_m Z_n}{\left|\vec{\tau}_m-\vec{\tau}_n\right|}$$

The kinetic energy term T is expressed as an UBER relation:

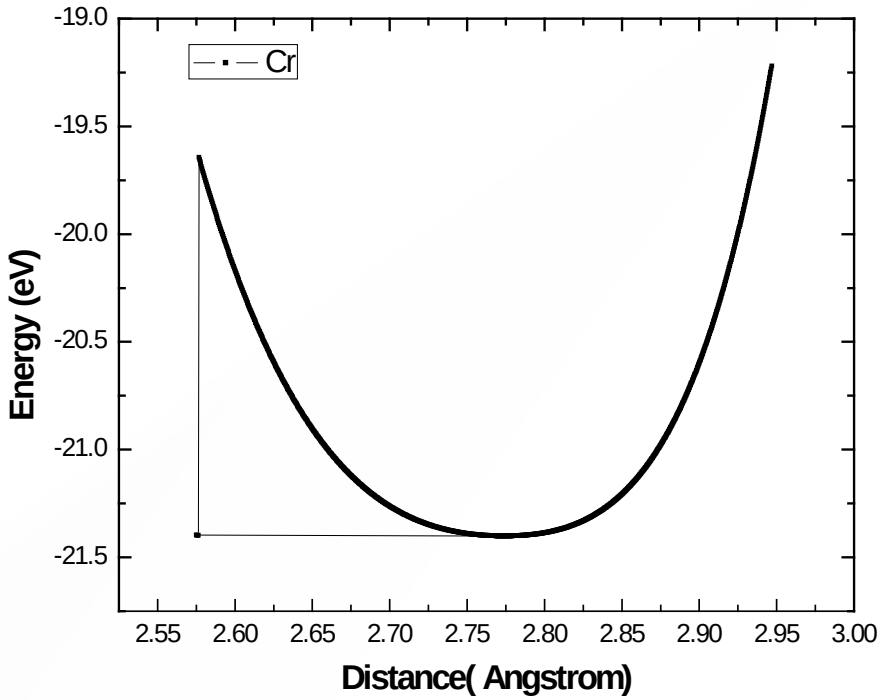
$$T \equiv E_{rep} = \frac{1}{2}\sum_{\substack{i,j\\(i\neq j)}} \varepsilon d_{ij}^{\,n} \exp\left(-\frac{d_{ij}-d_0}{s}\right)$$

Method

- **By fitting the coefficients in UBER relation into the total energy equation, we can calculate the total energy of the system, thus the interatomic potential is known.**

- **Then classical MD could be performed to simulate the physical properties.**

BCC Cr Total Energy ~ Distance



Predictive Tests

- Cu and Co systems were fully tested for lattice constants, bulk modulus prediction, and the results are in good agreement with those of experimental data. Cr, Y, and Cr-Y systems are finalizing.
- The vacancy formation energy of Cu is also tested. The BCC and FCC phase total energy results are consistent with experimental data.

Current Status

- **We have setup potentials for Cr and Y crystals. Cr-Y alloy system is finalizing.**
- ***Ab initio* MD simulation on Y, Mo, and W co-doped Cr alloy system had been finished.**
- **A test rig at LSU Turbine Innovation and Research (TIER) center is being tested for final oxidation and corrosion test.**
- **Pure Cr, Cr-Y (5%, 10%, and 20% Y) nanocrystal tests were done at LBNL beamline 12.2.2. %5 Cr-Y axial data had been analyzed, the rest radial data are processing by J. Lei and L. Tan.**

Cr-Y and Cr-Y-Mo-W System MD Simulation

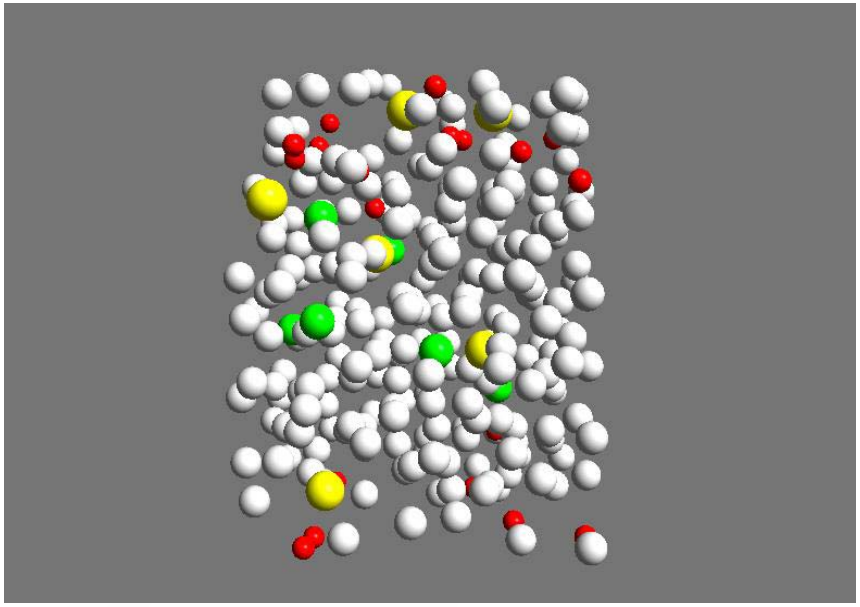
Different densities of Y-doping (Y/Cr)(2.5%, 5%, 14%) at different temperature: 1100K ~ 2100K

244 Cr 6 Y 2.5% soft at 2000K after 1.5 ns.

238 Cr 12 Y 5% stable solid at 1800K after 1 ns.

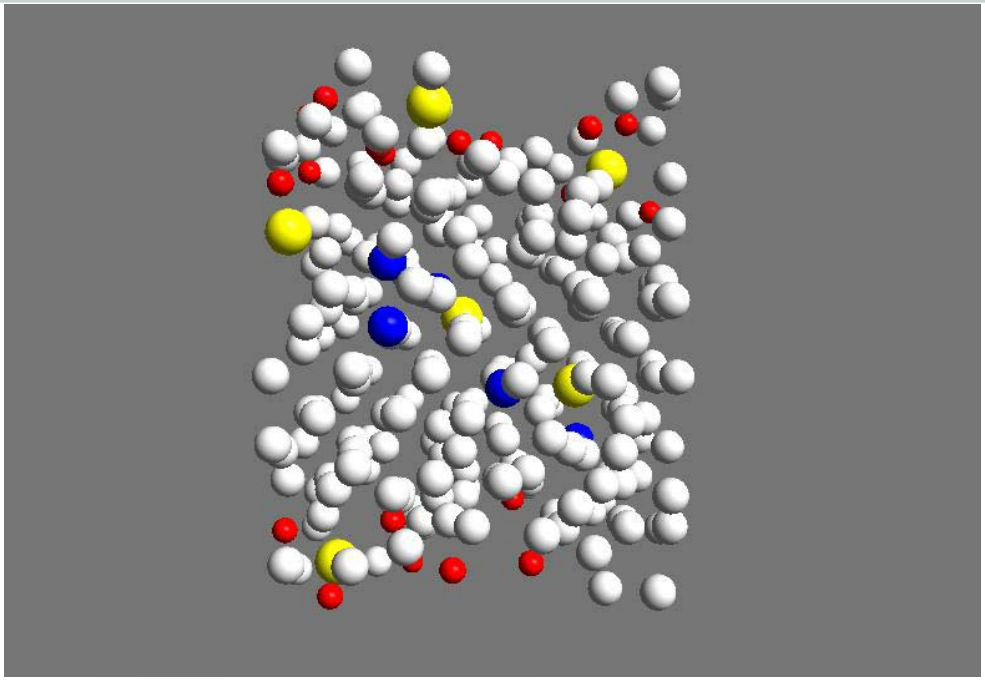
A cubic supercell consisting of 250 chromium atoms is set as 5×5×5. The dopants atoms (Y, Mo, W) are randomly dispersed to Cr bulk.

Cr-Y-W System at 1200K



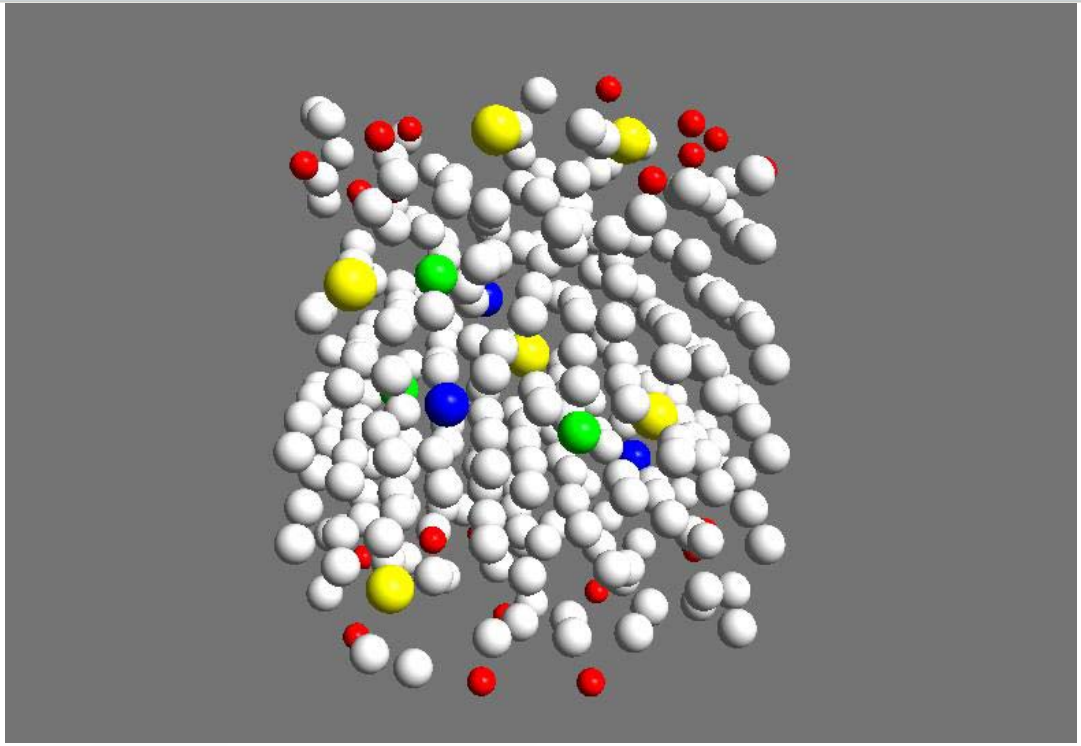
O/Cr-Y-W system at 1200 K with O atoms diffused. 238 Cr atoms (White), 6 Y atoms (Yellow), 6 W atoms (Green) and 21 O atoms (Red) are shown in the figure.

Cr-Y-Mo System at 1200K



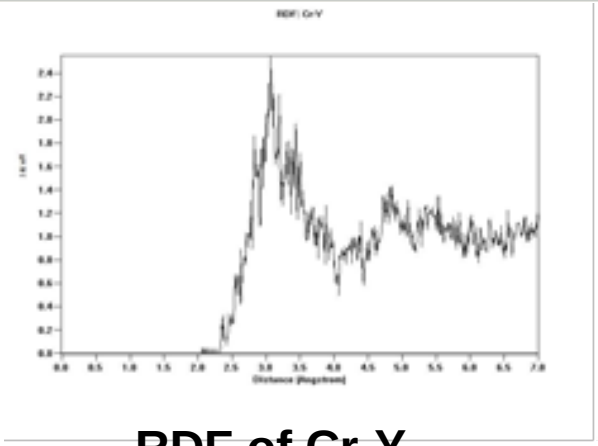
O/Cr-Y-Mo system at 1200 K with O atoms diffused. 238 Cr atoms (White), 6 Y atoms (Yellow), Mo atoms (Blue) and 21 O atoms (Red) are shown in the figure.

Cr-Y-Mo-W System at 1200K

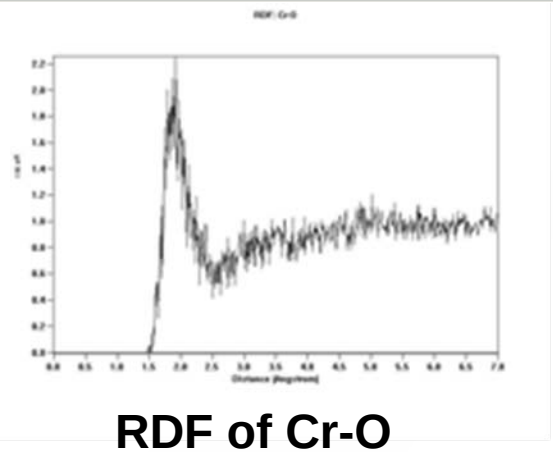


O/Cr-Y-Mo-W system at 1200 K with O atoms diffused. 238 Cr atoms (White), 6 Y atoms (Yellow), 3 Mo atoms (Blue), 3 W atoms (green) and 21 O atoms (Red) are shown in the figure.

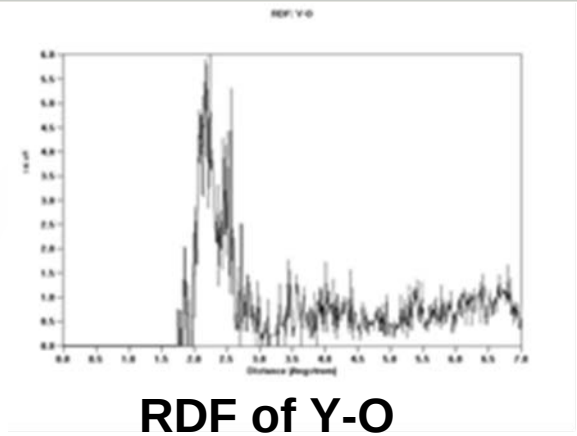
RDF analysis



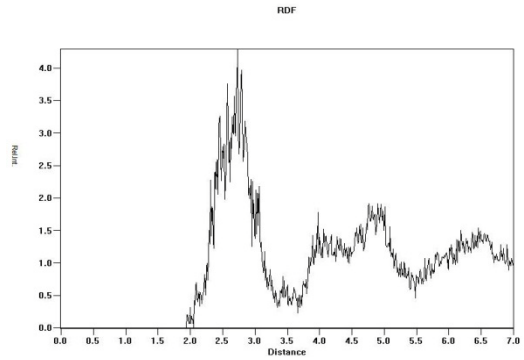
RDF of Cr-Y



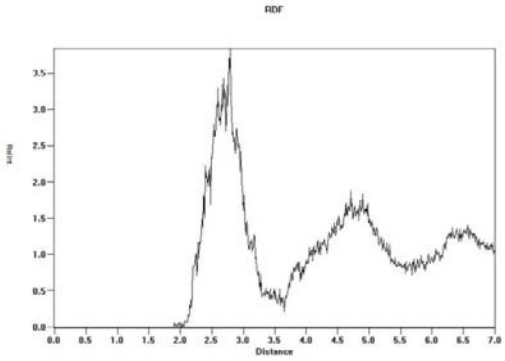
RDF of Cr-O



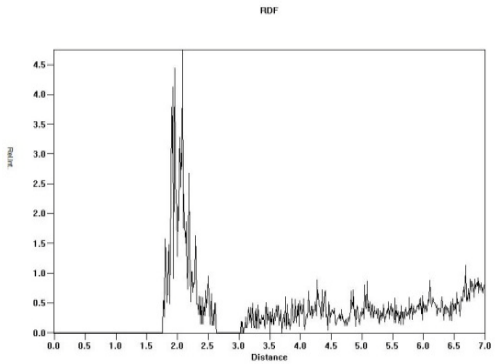
RDF of Y-O



RDF of Cr-Mo



RDF of Cr-W

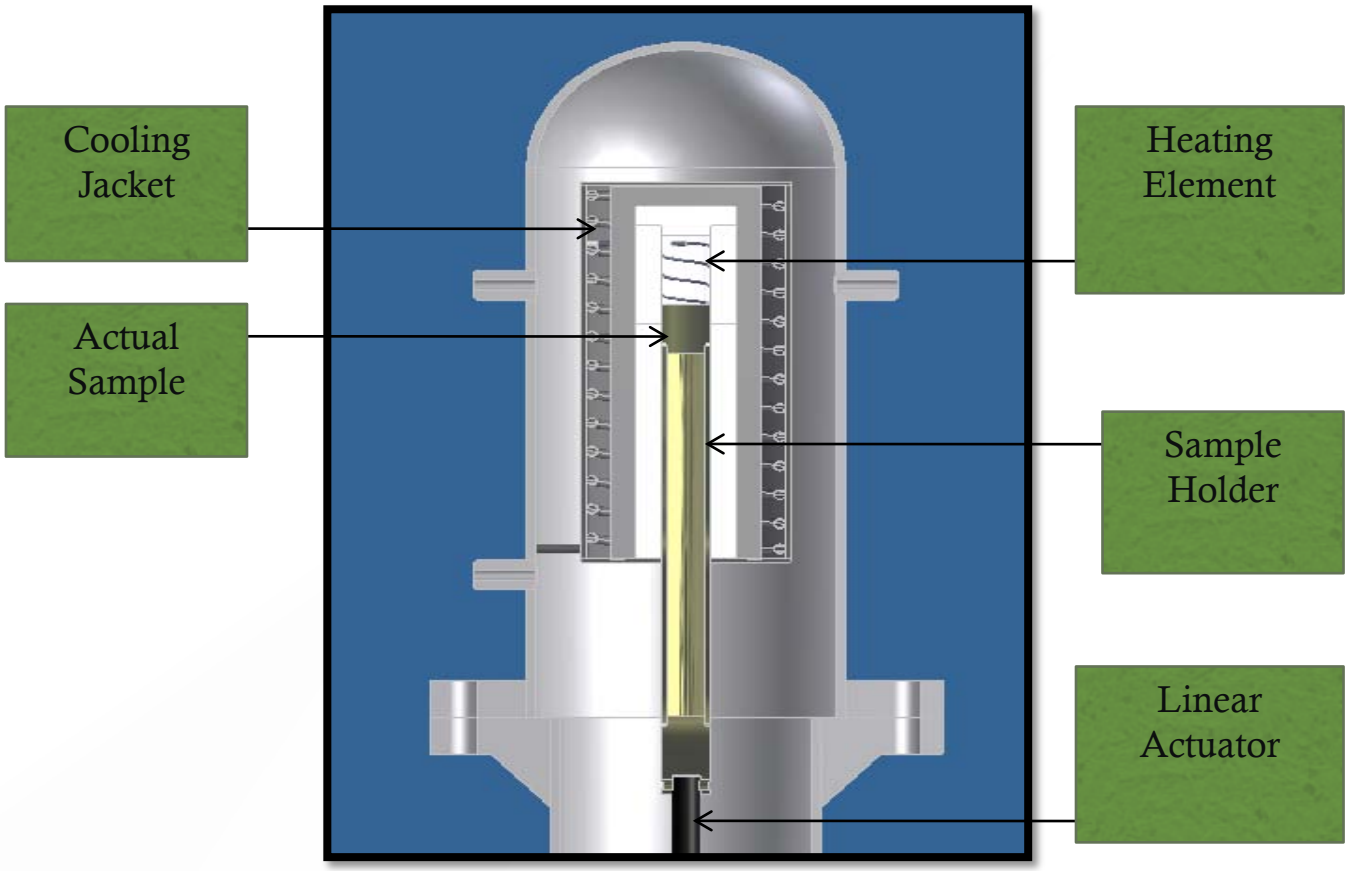


RDF of W-O

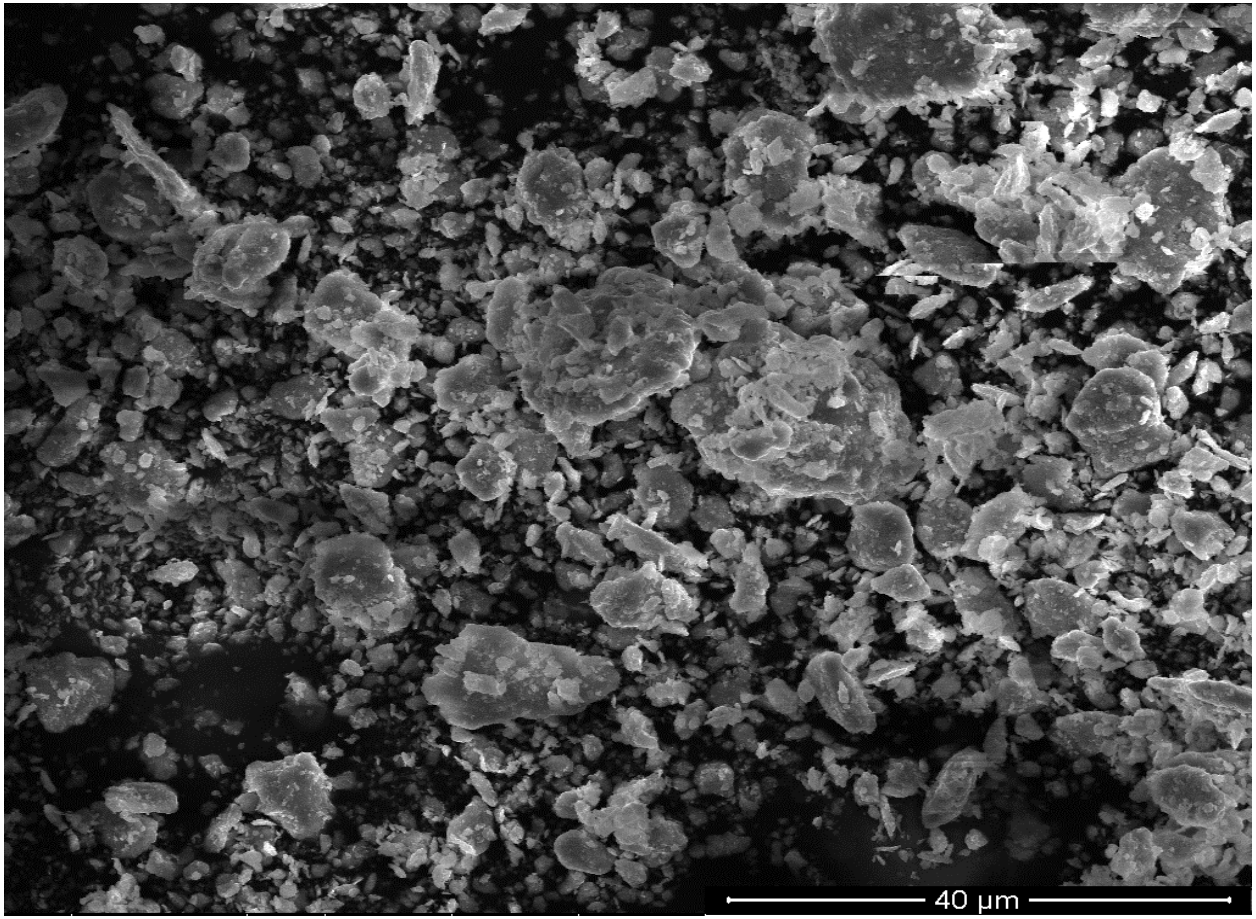
Cr-Y Alloy Experiment Performed

- The Cr-Y samples preparation (ball milling), SEM, and XRD are finished at LSU TIER.
- We have performed axial high pressure experiment (up to 36 GPa) on Cr-Y with wt 5% Y at LBNL beamline 12.2.2. The data had been processed. The results are combined with simulation data to be submitted for journal publication.
- The pure Cr, 20%Y doped Cr nanocrystal synchrotron radial tests had been finished in May 2012. The data processing is ongoing.
- The oxidation test rig is being tested for final oxidation experiment.

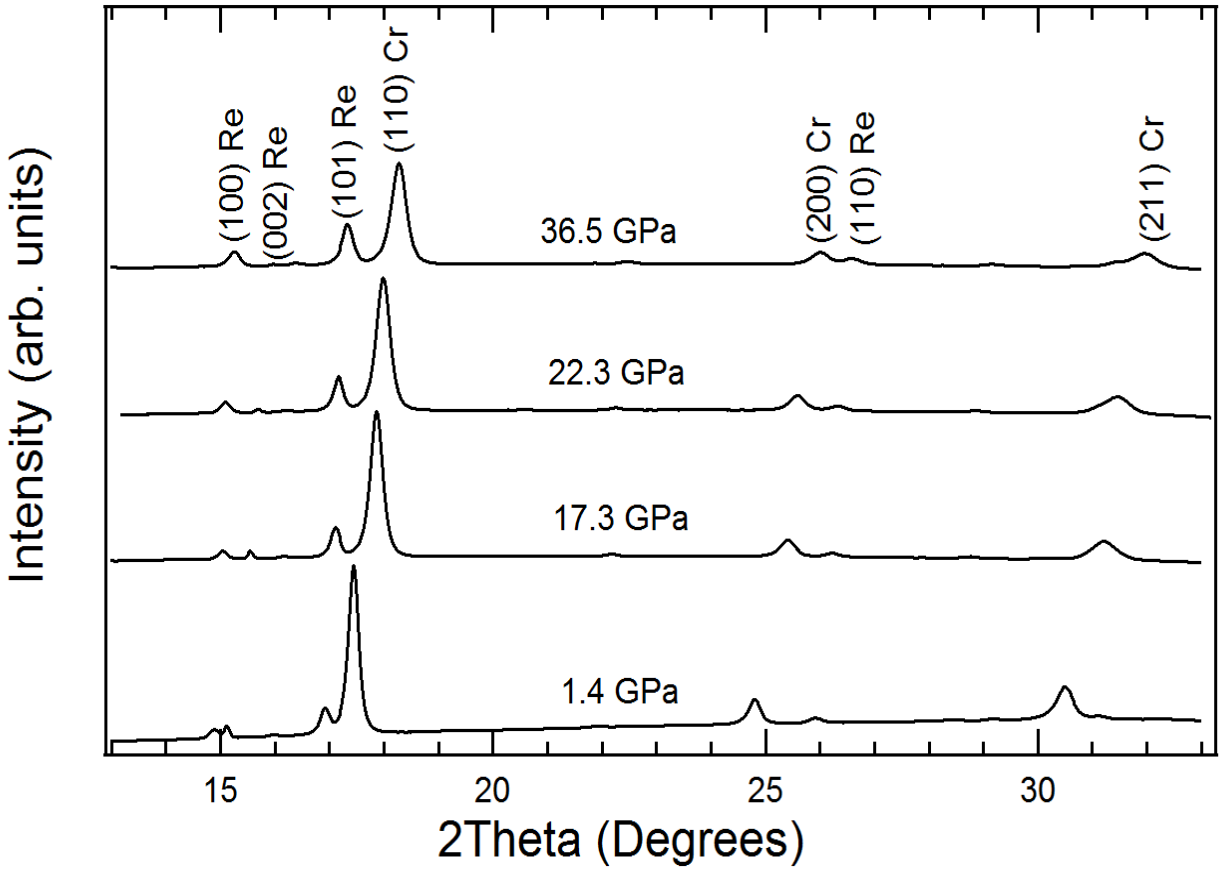
Testing Rig at LSU TIER (~1300 °C)



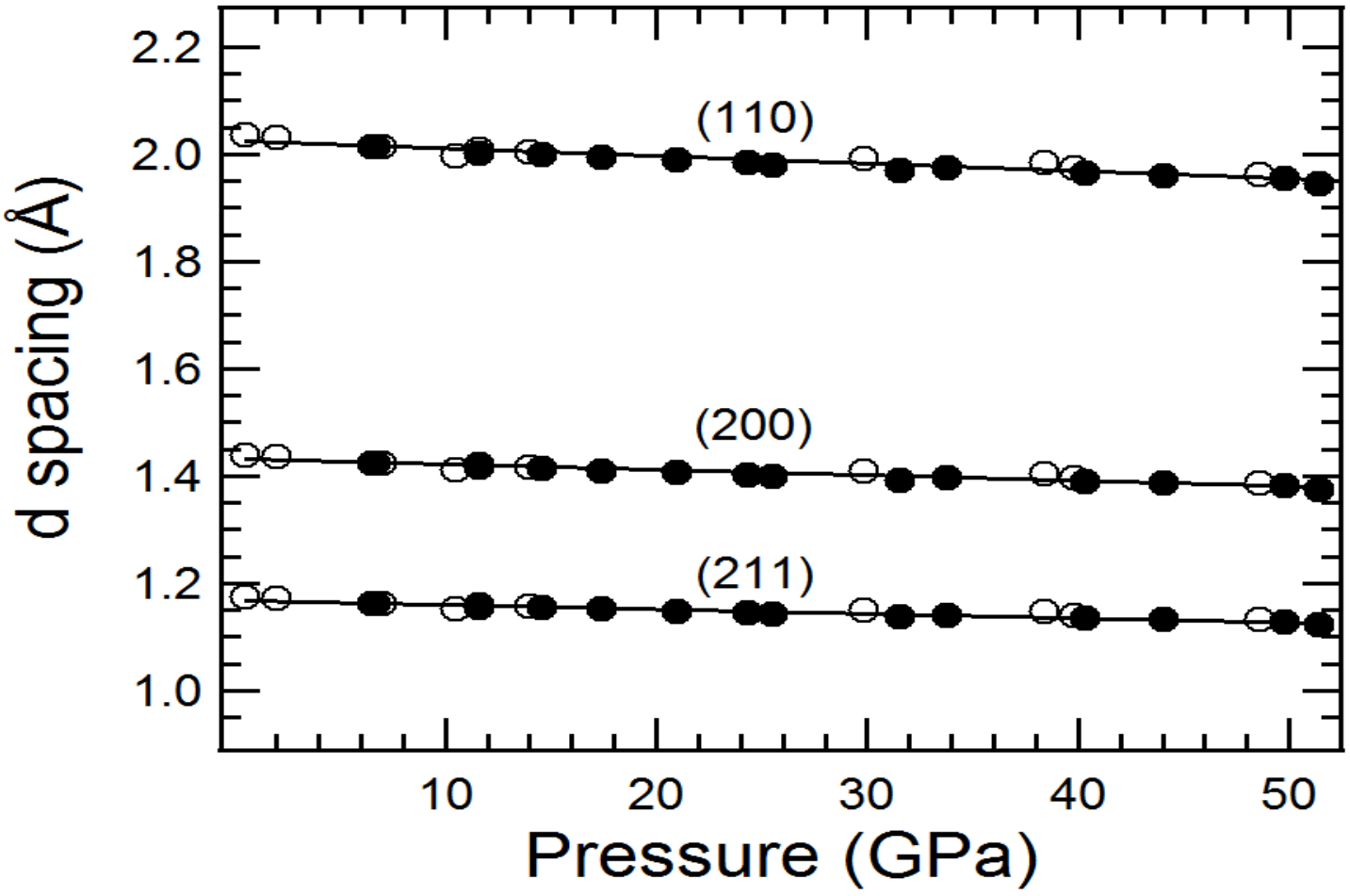
5%Y doped Cr SEM



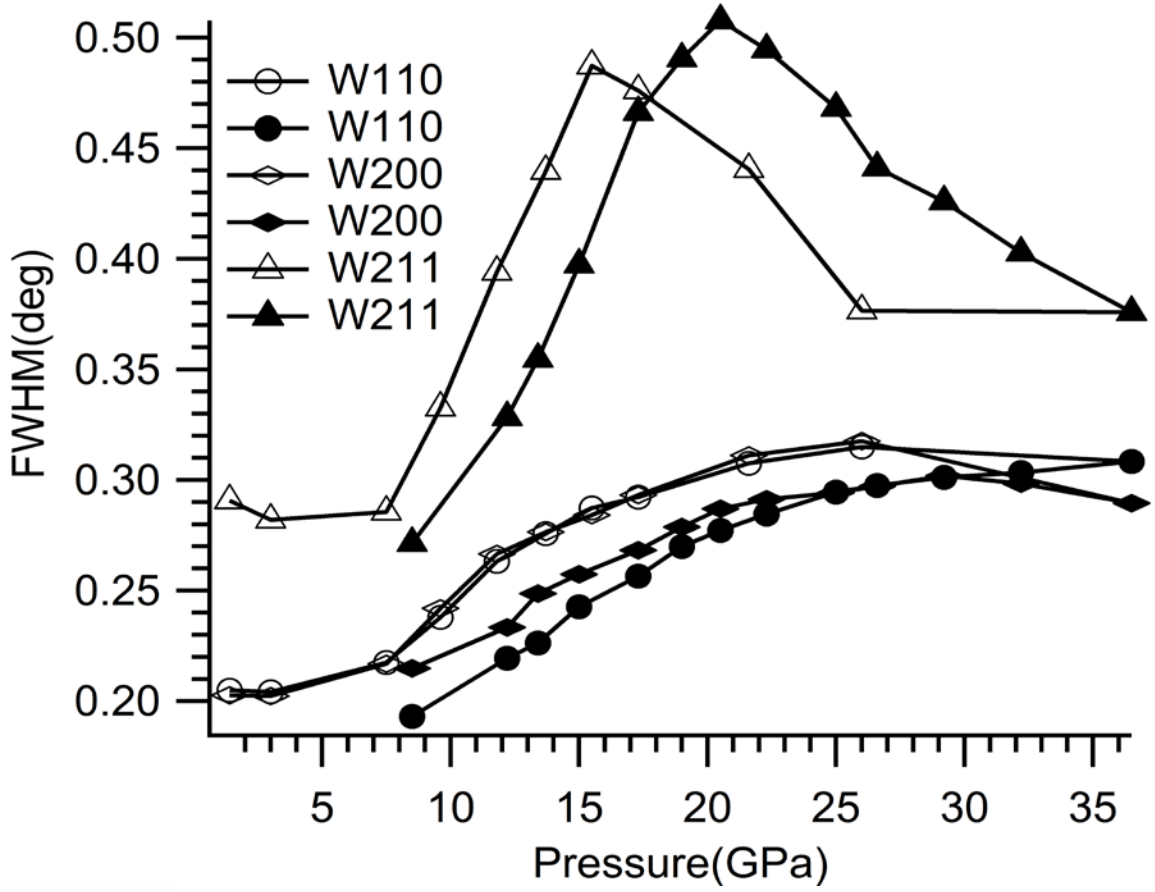
Pressure ~ Structure Relation



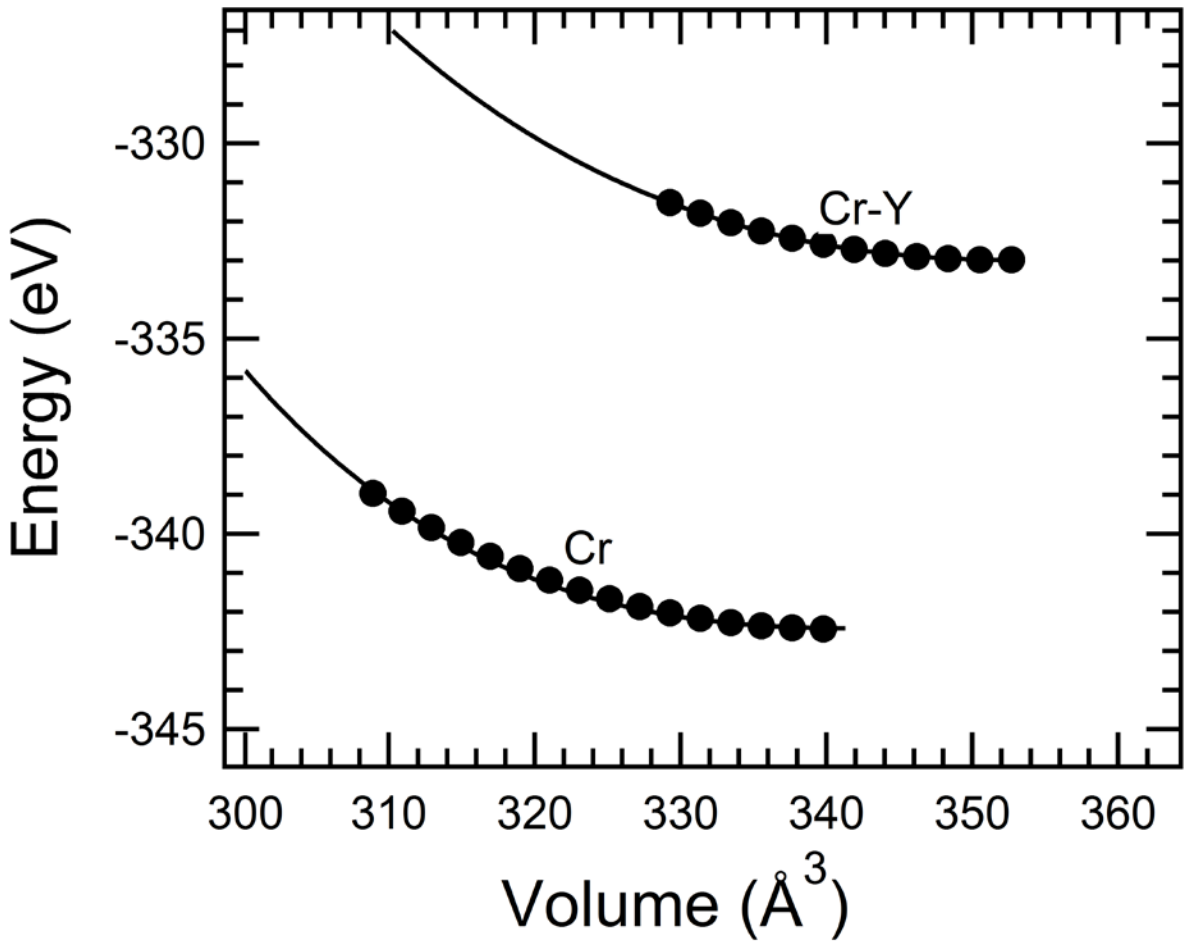
Pressure ~ d Spacing Relation



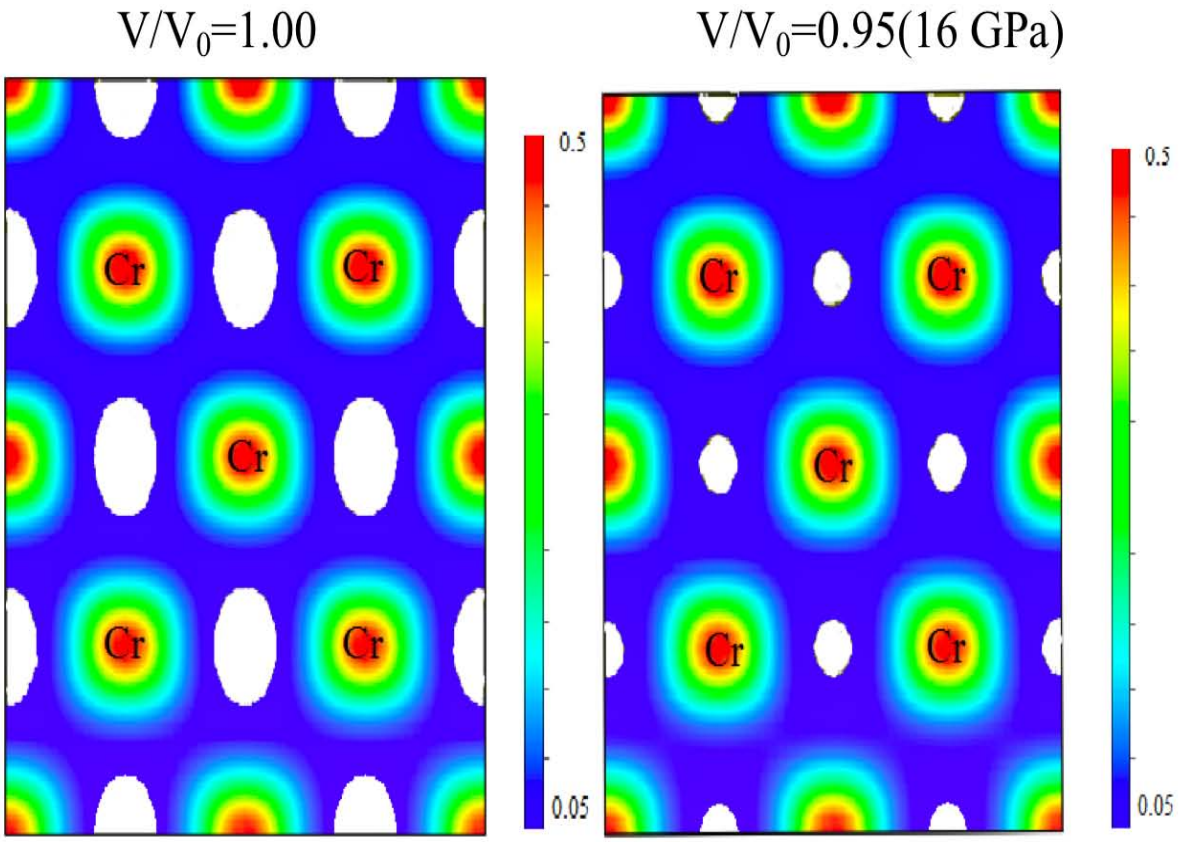
FWHM ~ Pressure Relation



Simulated Compression E ~ V

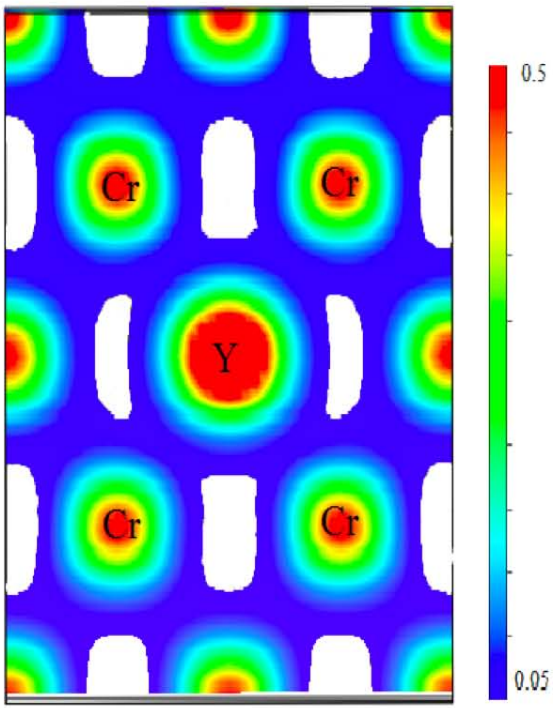


Pure Cr Charge Density

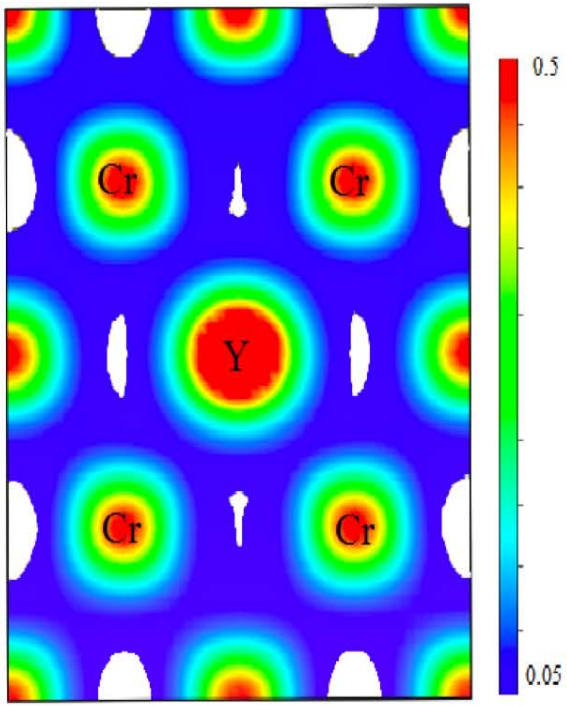


Cr-Y Charge Density

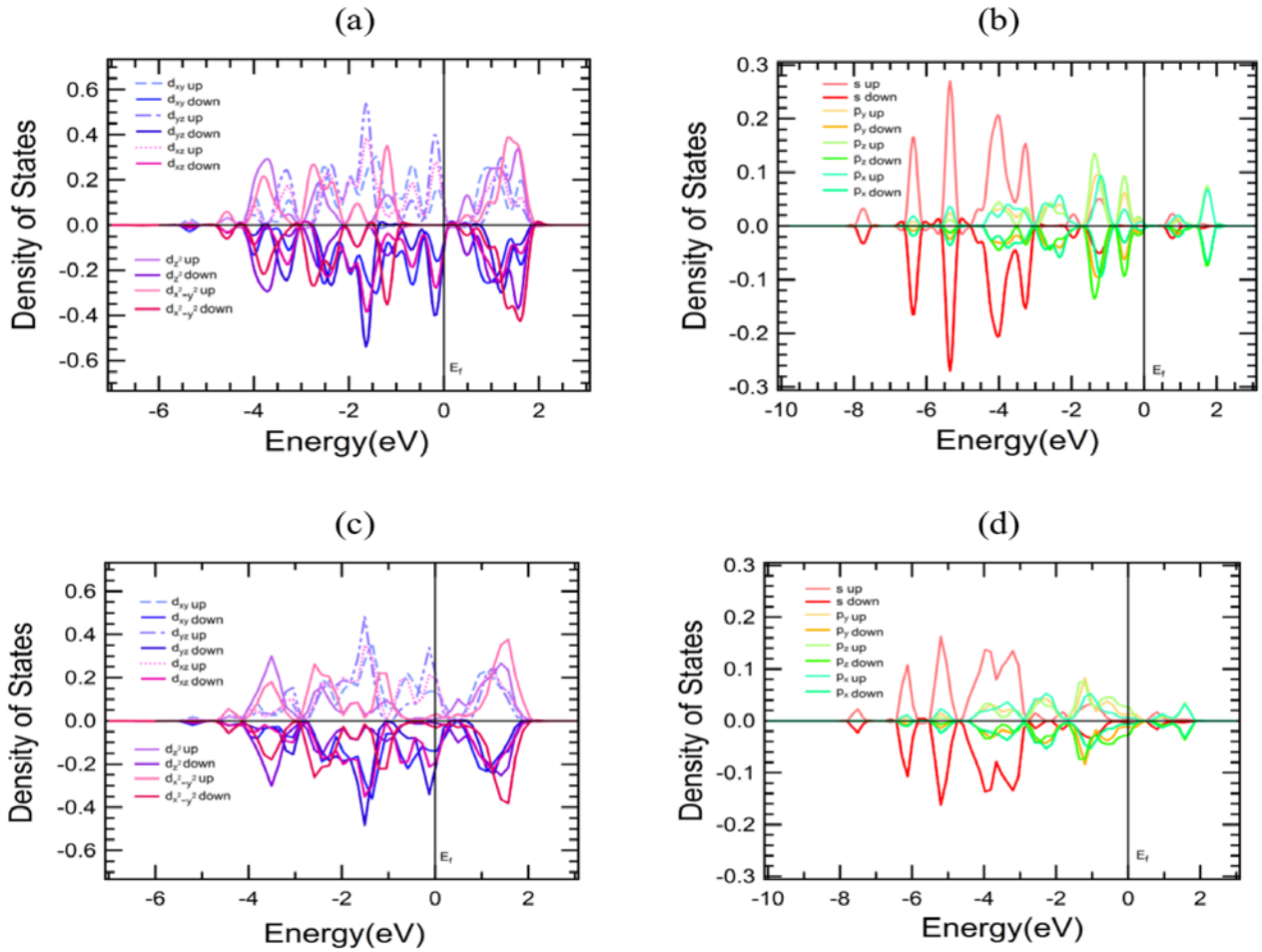
V/V_0=1.00



V/V_0=0.95(15GPa)

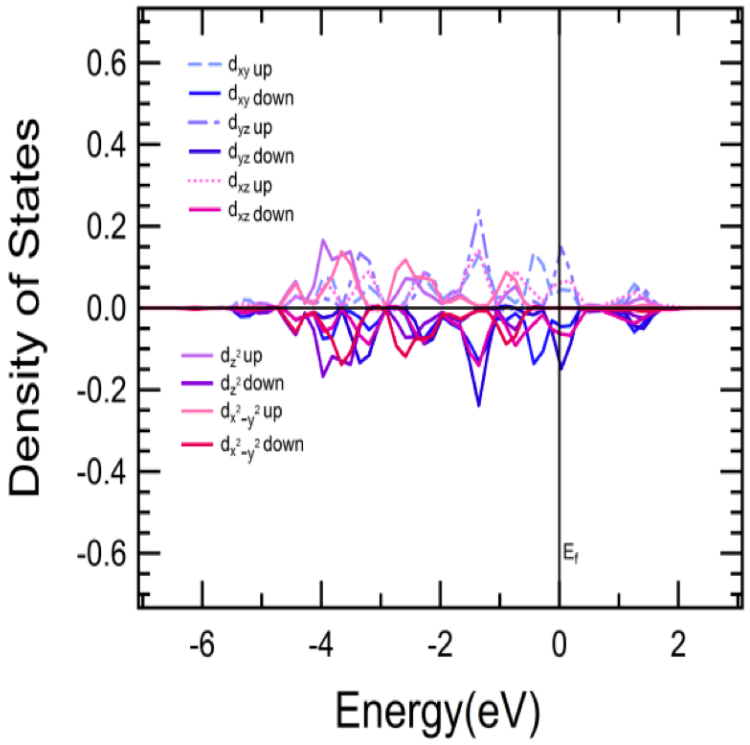


DOS: a/b-Pure Cr, c/d-Cr/Y

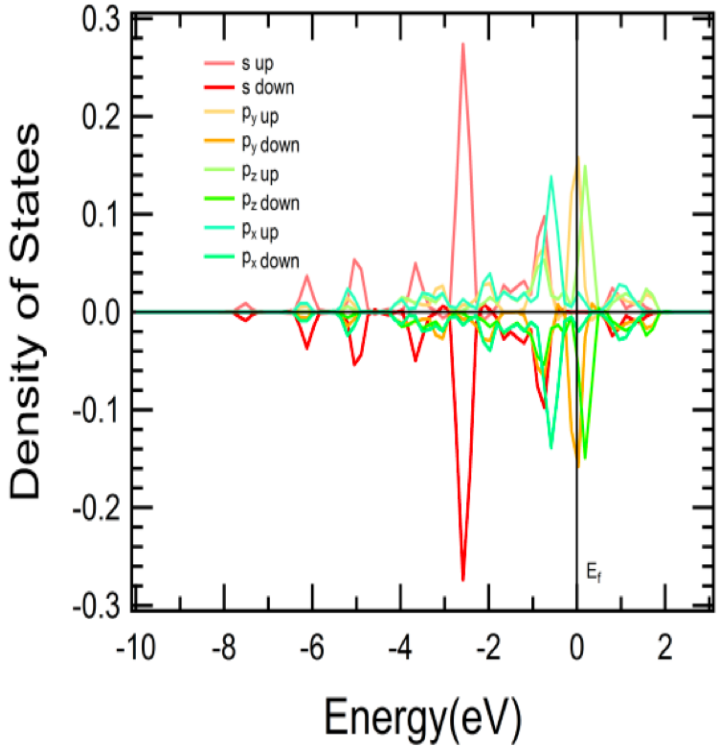


DOS: e/f-Y

(e)

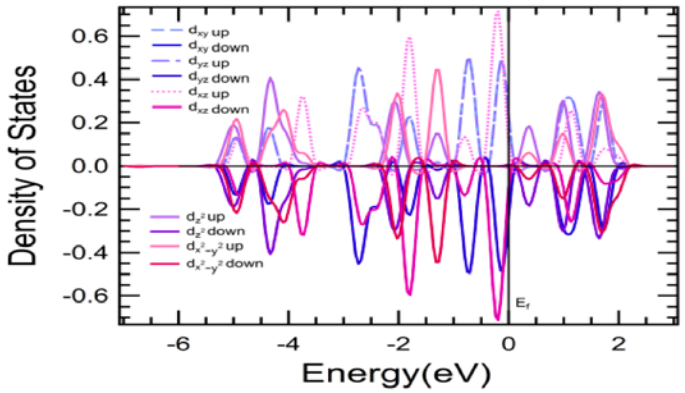

Density of States
Energy(eV)
E_f
d_xy up
d_xy down
d_yz up
d_yz down
d_xz up
d_xz down
d_z² up
d_z² down
d_x²-y² up
d_x²-y² down

(f)

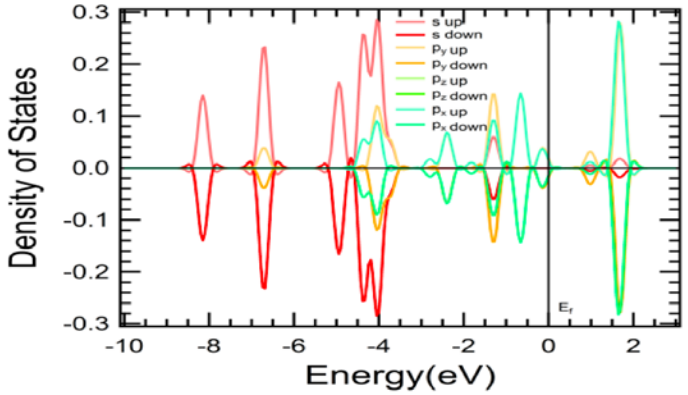

Density of States
Energy(eV)
E_f
s up
s down
p_y up
p_y down
p_z up
p_z down
p_x up
p_x down

Compressed DOS: a/b-Pure Cr, c/d-Cr/Y

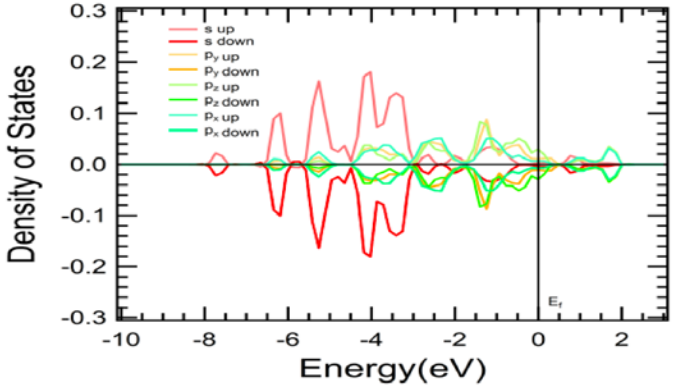
(a) V/V_0=0.95(16GPa)



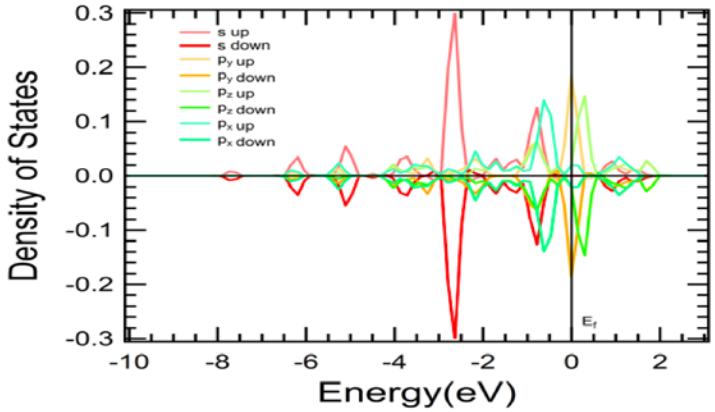
(b) V/V_0=0.95(16GPa)



(c) V/V_0=0.95(15GPa)



(d) V/V_0=0.95(15GPa)



Cr-Y(5wt%) Results

- Charge density analysis shows that the Y atom loses 0.3 electron to the nearest neighboring Cr atoms.
- Density of states calculation indicates *dsp* hybridation between Y and Cr atoms.
- The FWHM broadening at (211) shows a main plastic stain exists, while the data at (110) plane shows it is a slip plane.

Future Work

- Continue to test the Cr-Y and Cr-Ta interatomic potentials and compare the results with experimental data or pure *ab initio* ones if the experimental data does not exist.
- Improve the parallel MD code, set up Cr-Y and Cr-Ta models and perform *ab initio* HPC simulation.
- Experimentally validate the predicted potential high performance high temperature alloys. We will test Cr-Y and Cr-Ta alloys, perform microstructure analysis, and do oxidation and corrosion resistance test.

Acknowledgement

- Graduate students: Lei Zhao, Jialin Lei, Rui Guo, Rui Yao, Corey Baham, and Vani Panguluri.
- Postdocs: Drs. Liuxi Tan, Oleg Starovoytov.
- Drs. S. Guo, G. L. Zhao, E. Khosravi, K. Wang, Bin Chen.
- LONI Institute for supercomputer time and internal support.
- DOE NETL, NASA, NSF-LASiGMA, and NIH-INBRE funding support.