

Molecular Dynamics Simulation and Experimental Validation on Cr-based Alloys

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6/7/2011 Pittsburgh, PA



Outline

Introduction

Method

Cr-based Alloy Simulation and Experiment

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.

- Use Cr-Y as a model system to test a novel *ab initio* molecular dynamics (MD) method for new high temperature refractory metal alloy simulations.
- Experimental validation on the simulation results.

Previous Works on Cr-Y Alloy

Theoretical work:

1. Density function theory (DFT) with full-potential linearized augmented plane wave (FLAPW) method
2. Studied $4d$ element Y doped dilute Cr-Y alloy: magnetic hyperfine fields of impurity in Cr-host.

S. N. Mishra, Phys. Rev. B **77**, 224402 (2008).

Previous Works on Cr-Y Alloy

Experimental work:

1. Oxidation behavior study on Yttria addition of 0.5 ~4 wt.% mechanically alloyed Cr-based alloy.
2. Strong suppression on Cr_2O_3 -scales in Cr-Y alloy was observed. The distribution of Y plays an important role.

U. v. d. Crone, M. Hänsel, W. J. Quadakkers, and R. Vaßen,
Fresenius J. Anal. Chem. **358**, 230 (1997).

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.**

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

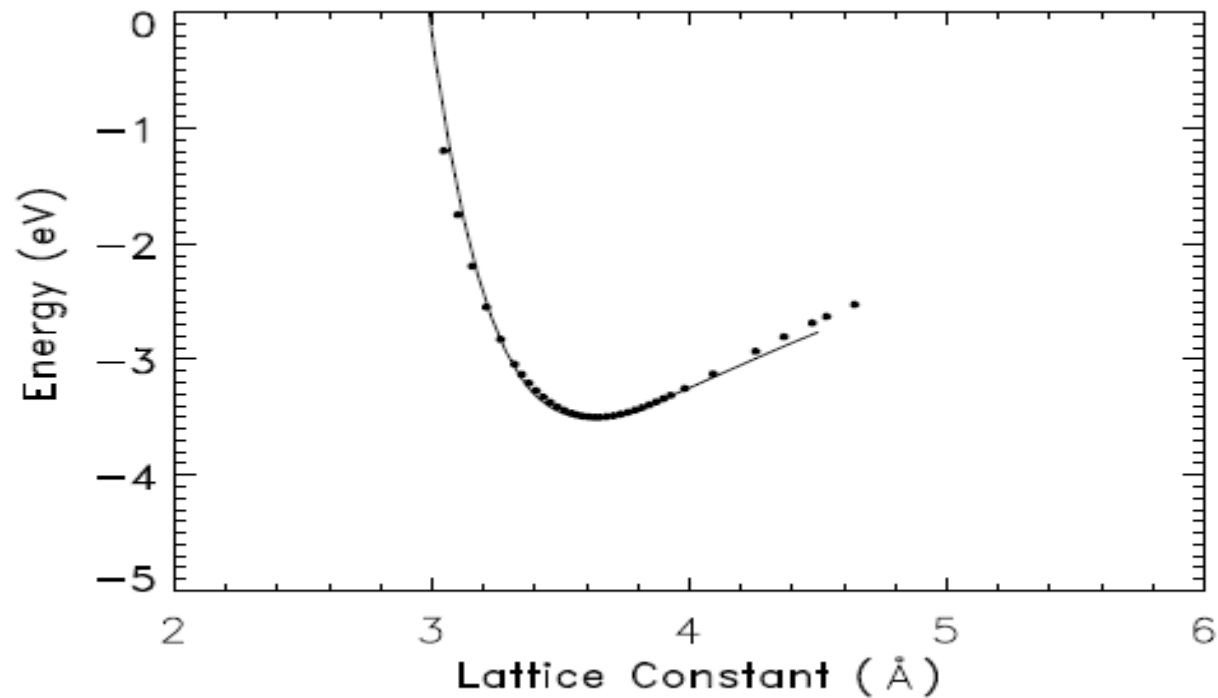
The kinetic energy term T is expressed as an UBER relation:

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

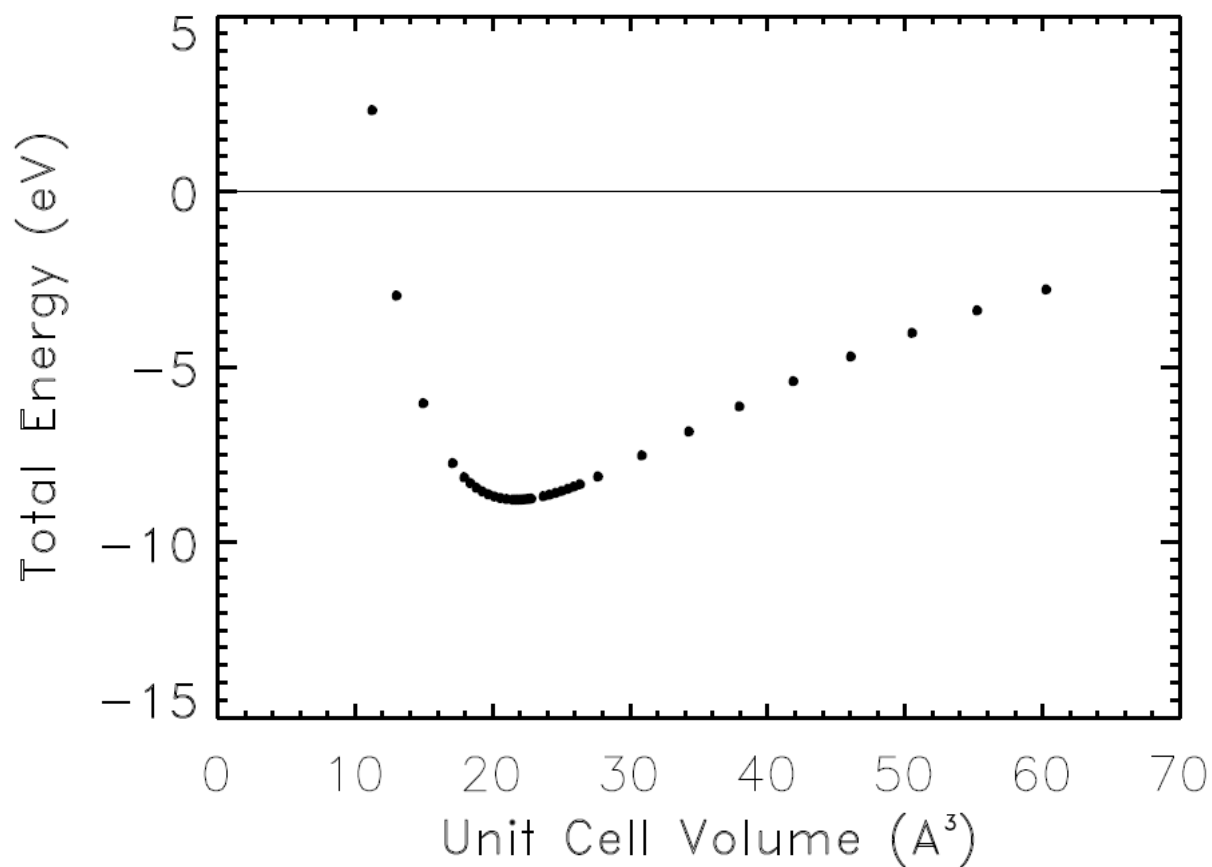
Method

- **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.**

FCC Cu Model System Total Energy



HCP Co Model System Total Energy



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.**
- **The vacancy formation energy of Cu is also tested. The BCC and FCC phase total energy results are consistent with experimental data.**

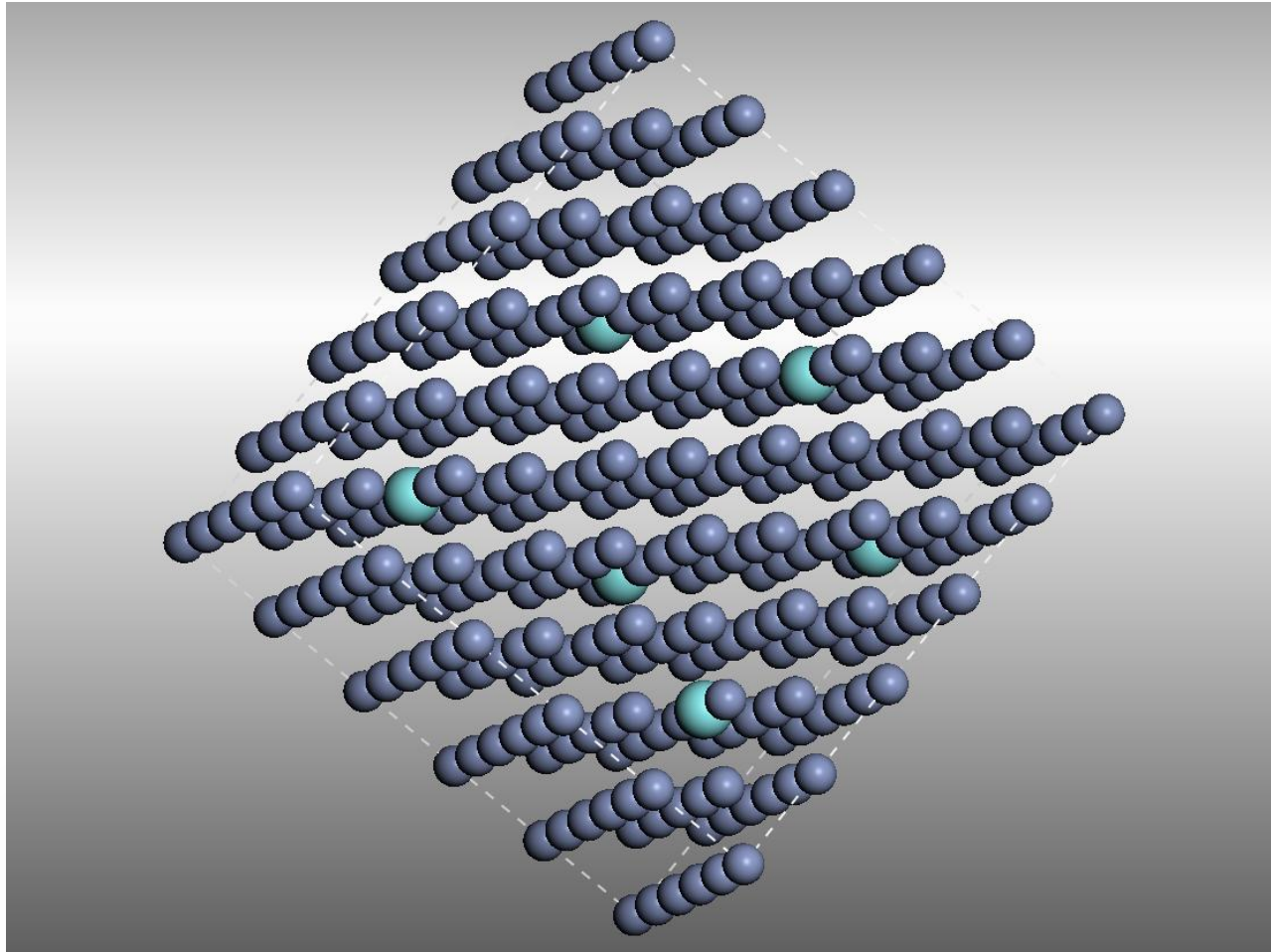
Current Status

- We have setup potentials on Cr and Y crystals.
- A comparison Cr-Y system *ab initio* MD simulation had been finished.
- A test rig is set up at LSU Turbine Innovation and Research (TIER) center.
- Cr-Y crystal test is done at LBNL beamline 12.2.2.
- Currently, we are working on Cr-Y system potentials and MD code parallelizing test.

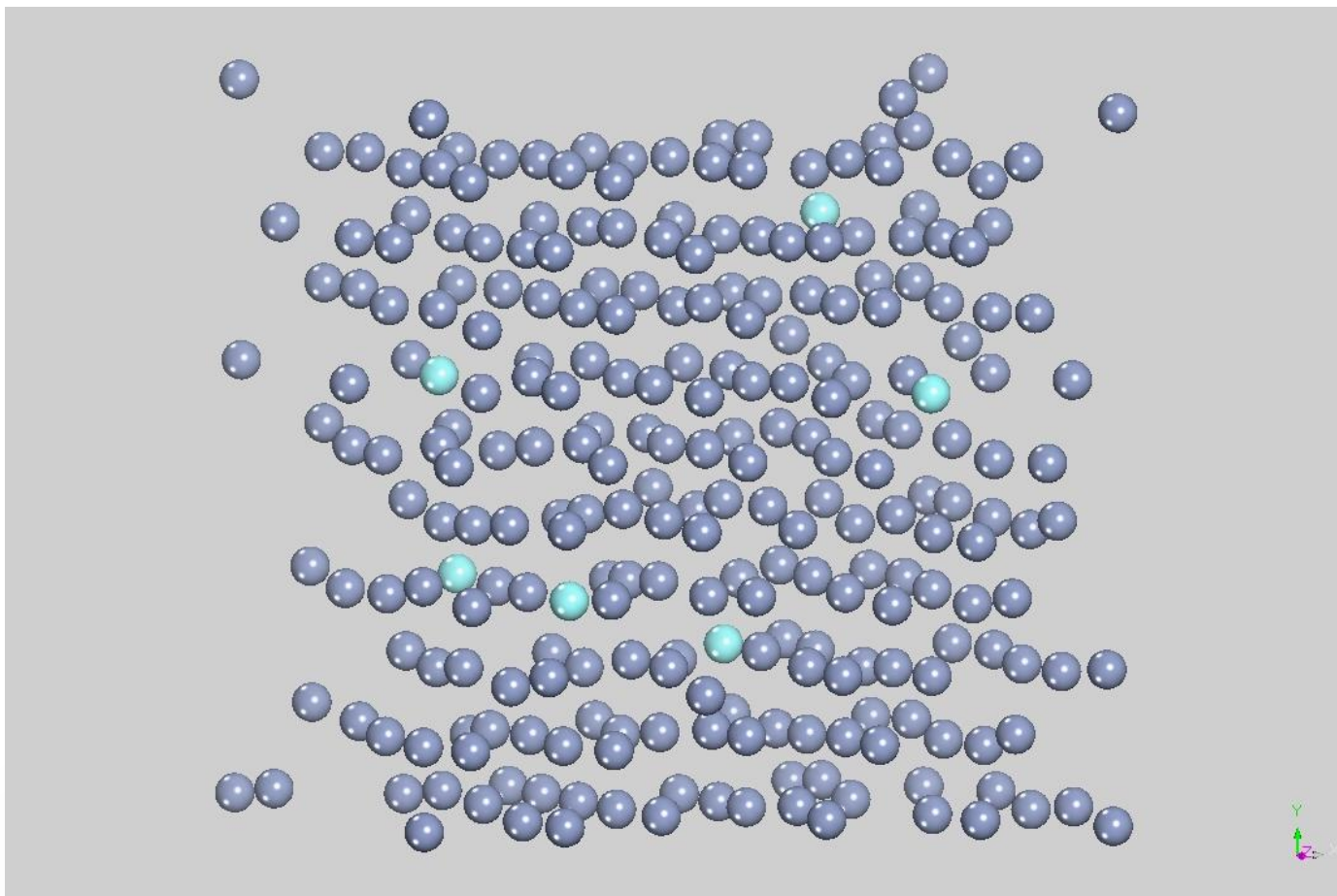
Cr and Y *ab initio* Results

- For Cr, with 600eV plane wave cutoff and total 220 irreducible k-points in the unit cell we got the lattice constant 2.78 Å (T= 0K). The experimental value is 2.88 Å (T = experimental value).
- For Co and Y crystals, we got the c/a ratio 1.62 (exp. 1.62) and 1.56 (exp. 1.57) respectively with 400 eV planewave energy cutoff at T= 0K.

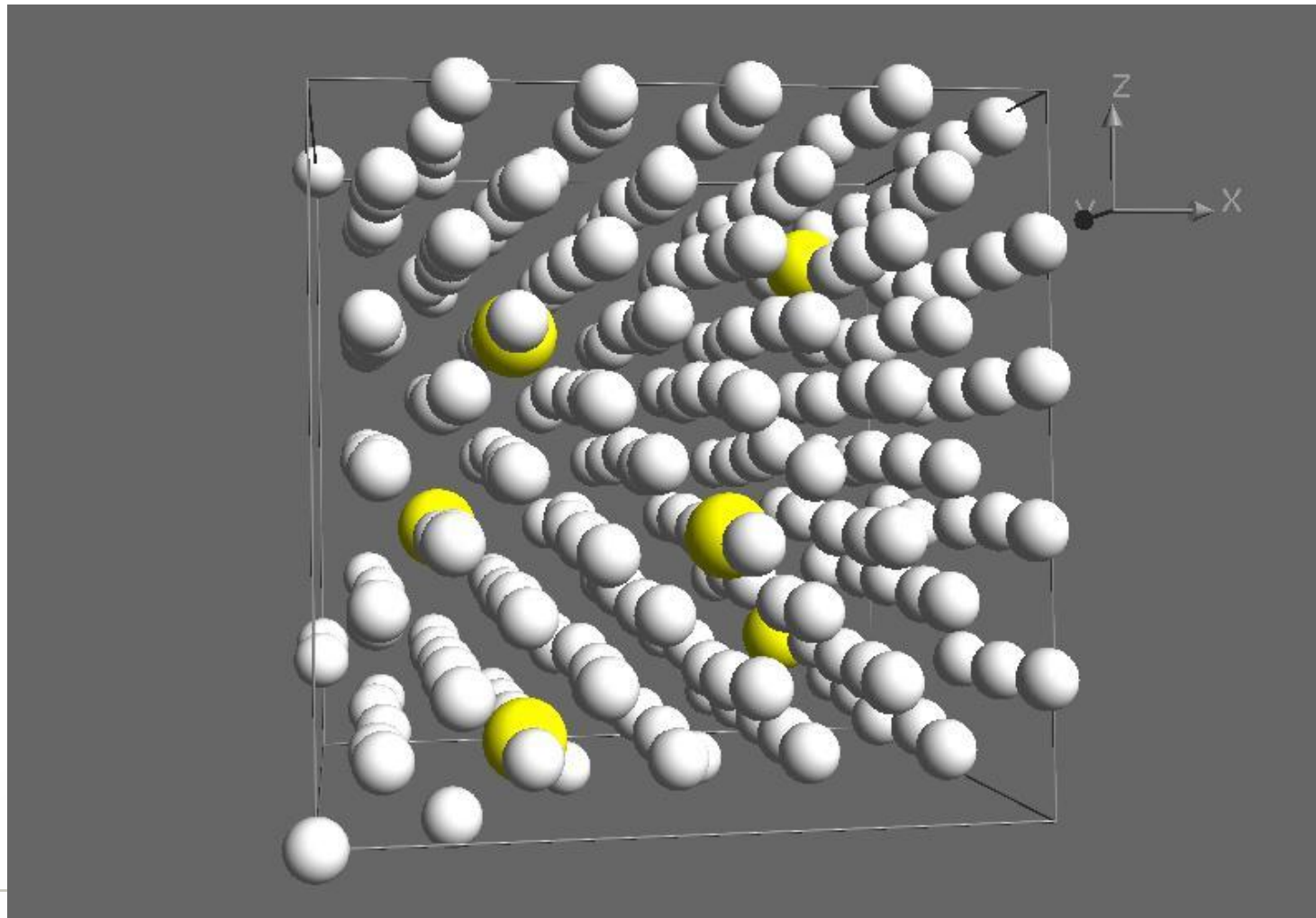
Cr-Y (244:6, 2.5% at Initial State)



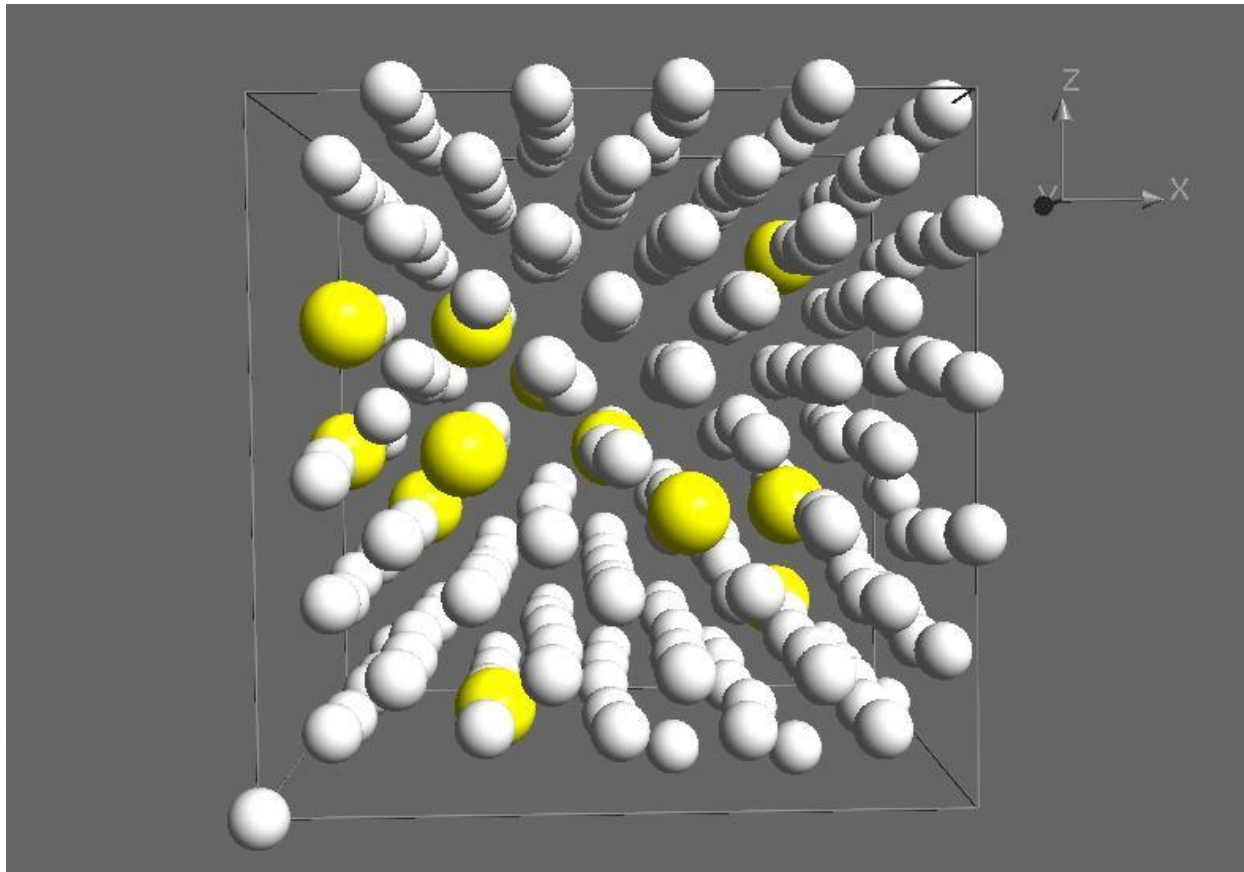
Cr-Y (244:6, 2.5% at 2000K 1.5 ns)



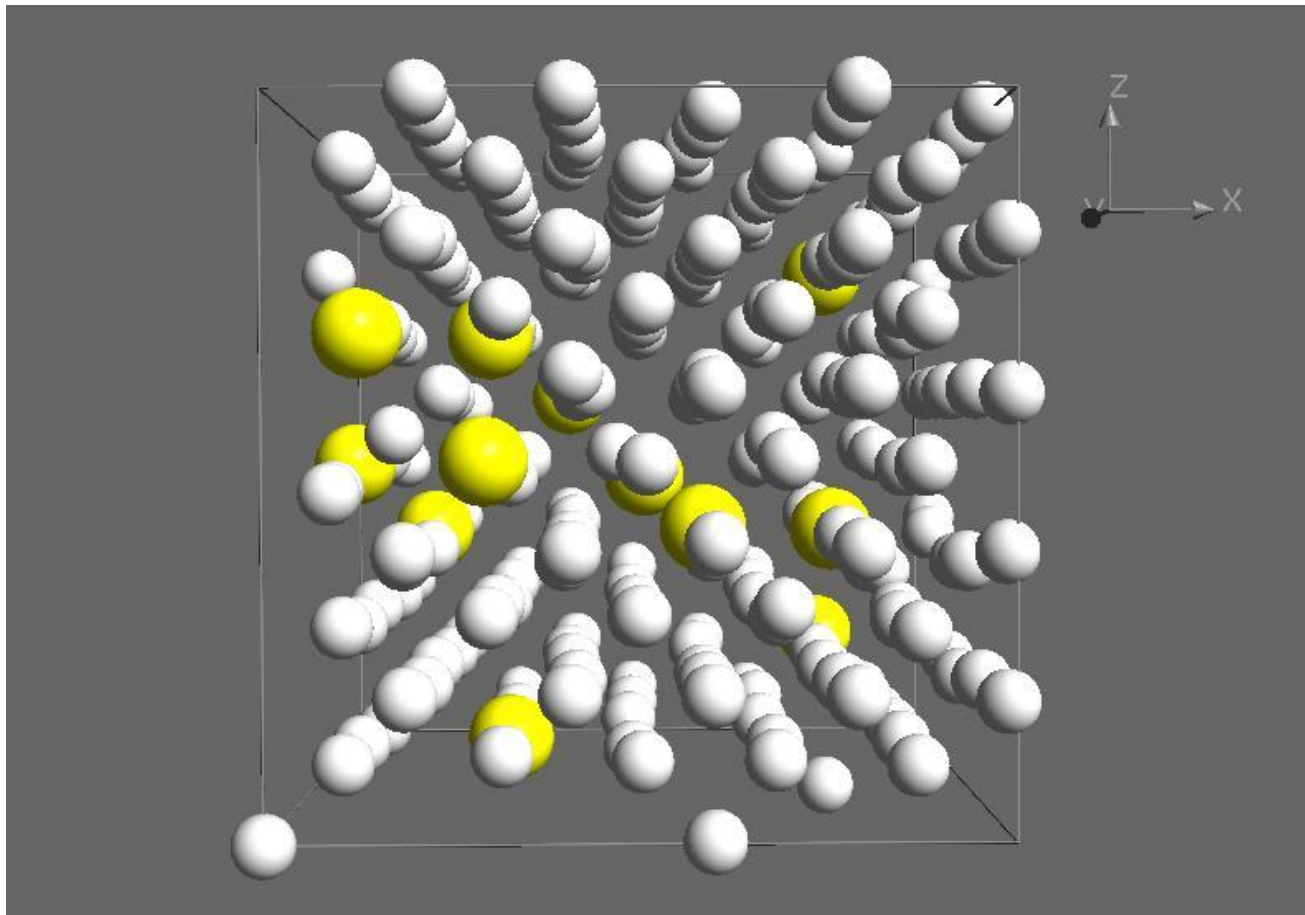
Cr-Y (244:6 2.5% at 1500K 1 ns)



Cr-Y (238:12, 5%at 1700K 0.5 ns)



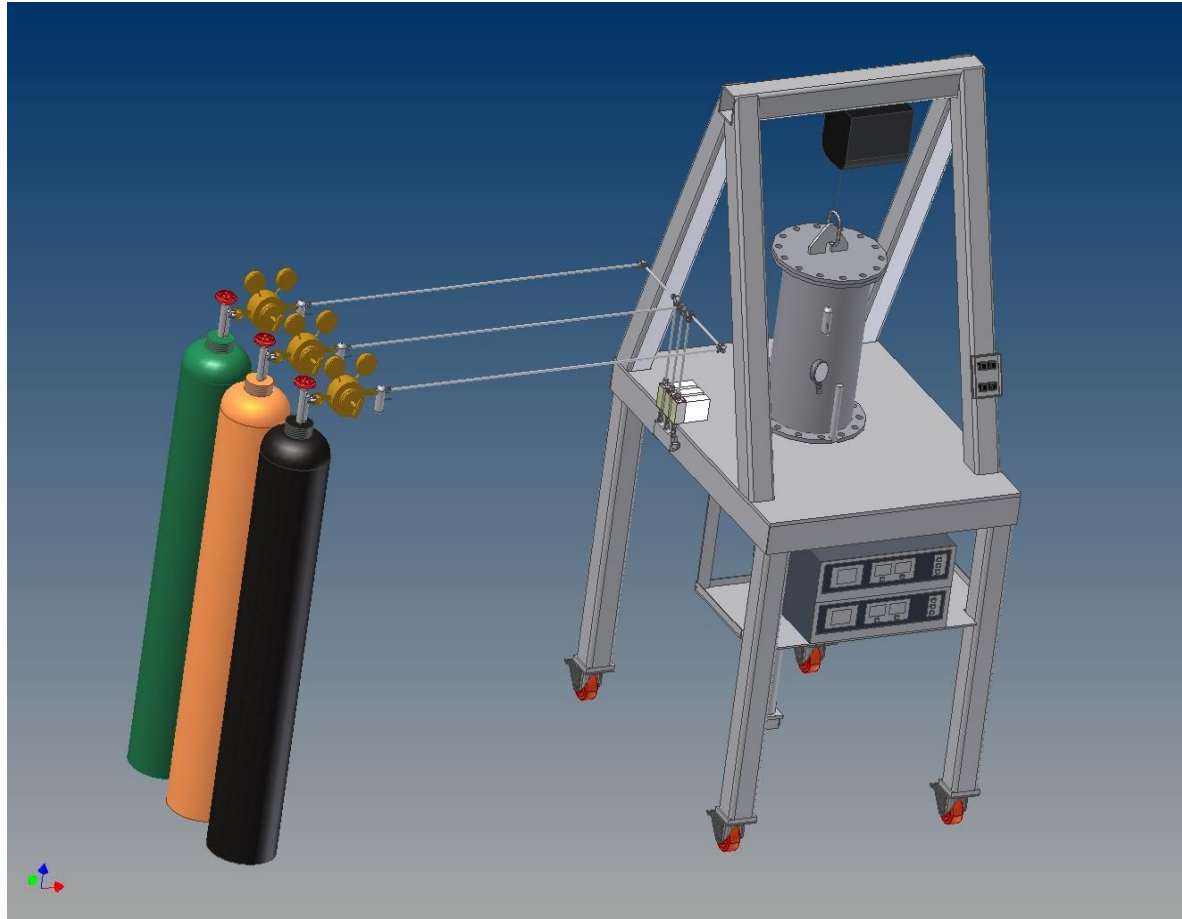
Cr-Y (238:12, 5% at 1800K 0.5 ns)



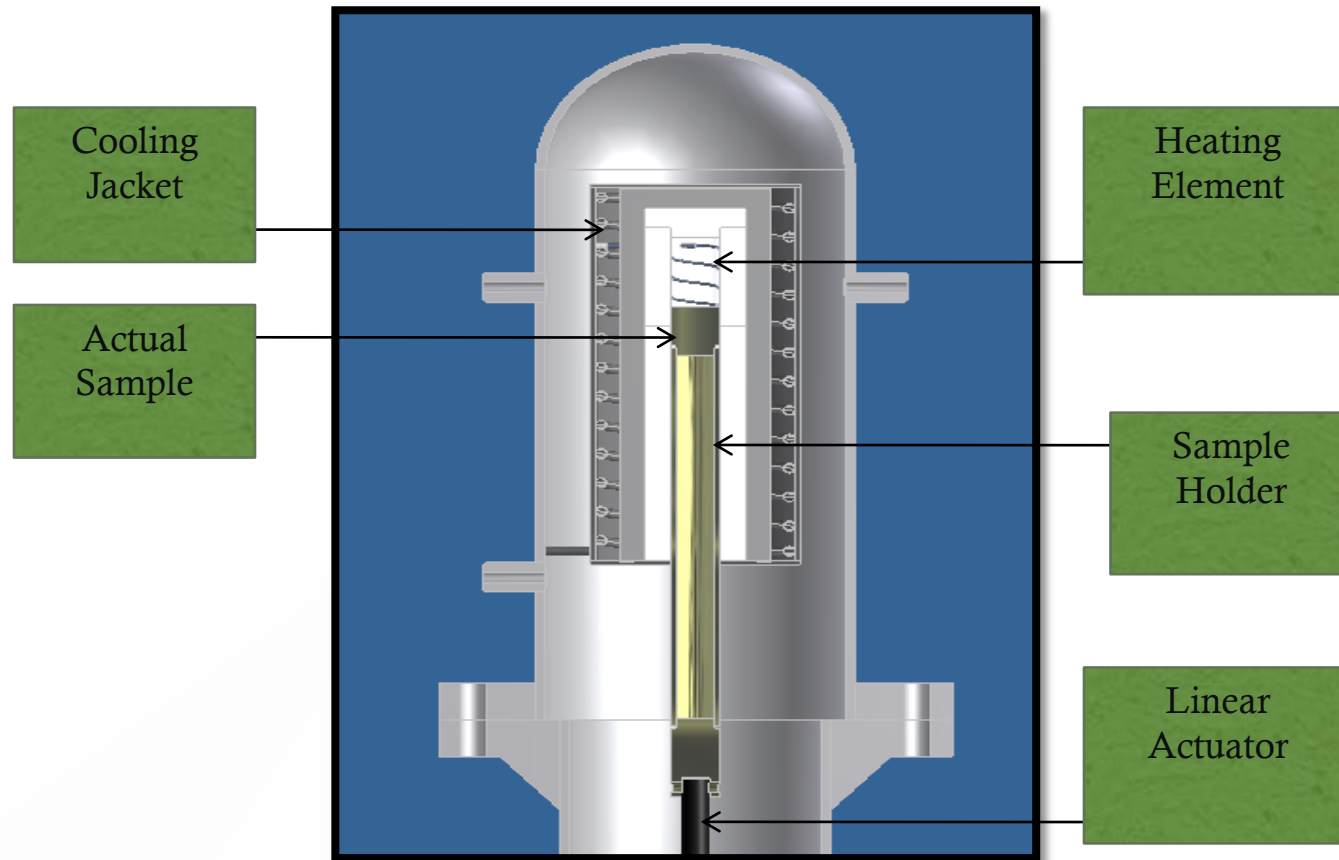
Cr-Y Alloy Experiment Performed

- We have performed axial high pressure experiment (up to 42 GPa) on Cr-Y with wt 5% Y at LBNL beamline 12.2.2. The data is currently under processing.
- The Cr-Y samples are prepared at LSU TIER with ball milling.

Testing Rig at LSU TIER (~1300 °C)



Testing Rig at LSU TIER (~1300 °C)



Future Work

1. **Cr-Y, Cr-O, and Y-O potentials for high temperature oxidation resistance simulation.**
2. **Cr-S, and Y-S potentials for high temperature corrosion simulation.**
3. **Cr-Ta, Ta-O, and Ta-S potentials setup and test.**
4. **Experimental verification on the high temperature oxidation and corrosion results.**

Acknowledgement

- **Graduate students: Lei Zhao, Jialin Lei, Rui Guo, Rui Yao, Corey Baham, and Vani Panguluri.**
- **LONI Institute for supercomputer time and internal support.**
- **DOE, NASA support.**
- **Drs. S. Guo, G. L. Zhao, E. Khosravi, K. Wang, Bin Chen.**