NE795 Fall 2021 Final Project Notes

What is the effect of +U on elastic constants of FCC U?

Convergence study on cutoff energy

Convergence study on kpoint mesh

U=0, 1, 2, 3, 4

Spin polarized

**Mahmoud: Grade: 75**

**Grade notes: -15 for 3 day late delivery;**

While I appreciate the effort in the motivation/introduction, FCC is considered a purely theoretical phase of U. This exercise was intended as academic in nature. Additionally, Crocombette’s work was on UO2, and while the U atoms in fluorite UO2 have a fcc lattice, he did not study pure FCC U.

You don’t specify your supercell. Are you using a single unit cell? That is not required.

Your kpoint testing was done with a cutoff energy of 39 eV? This must be Rydberg.

The number of kpoints in a 4x4x4 mesh is not 4. If symmetry is removed, it is 64. With symmetry, it depends upon that symmetry

Your energy cutoff is in units of Rydberg, not eV.

Did you perform a volume optimization to get the equilibrium volume?

I had requested elastic constants, not just elastic modulus. Thus, I was looking for C11, C12, and C44. Also, a stress-strain curve in essence could be utilized, but for the bulk modulus, it is small strains to develop a pressure versus volume curve and taking the derivative of that curve to obtain the modulus. You seem to be after the Young’s modulus, which is going to require more strain and such a calculation is not suited for a single unit cell analysis.

You didn’t state how you obtained the Young’s modulus. Also, there is no reason why additional simulations would yield different results. This is not a temperature-based system with random fluctuations. Slight changes in the convergence could lead to changes in the resultant state, but not significantly so.

You should have asked more questions about the process and what was required to meet the goals of the project.

**Hamdy: Grade: 85**

**Grade notes: -5 for 1 day late delivery;**

Correct structure and process to obtain relaxed structure. You didn’t state what your relaxed lattice constant is. It looks like it is about 1 Å higher than I would have expected.

Appropriate energy cutoff convergence study, but what is the kpoint mesh used for the energy cutoff convergence study? It seems from your input files that it was 8x8x8…

You are not looking for the lowest energy in a convergence study, you are looking for the converged energy. The 1x1x1 kpoint mesh has the lowest energy, but due to the coarseness, there is error associated with that low value. By increasing the kmesh density, we see that the actual energy is higher than that predicted from the coarse kmesh.

I was looking specifically for the C11, C12, and C44 elastic constants, but yes the bulk modulus technically is an elastic “constant”. What is the magnitude of your displacement? Also, we think of the dP/dV curve as being quadratic in nature, not linear.

Also, I find it highly unlikely that the pressure difference is EXACTLY the same for all +U values. In fact, the equilibrium volume should change with +U. So, I assume that there must be something wrong here. Also, what is the value of the bulk modulus here?

Overall, you followed along the lines of what I was looking for, but didn’t quite get there.

**Khadija: Grade: 85**

**Grade notes: -5 for 1 day late delivery;**

Good description of problem setup and appropriate information for convergence testing of energy cutoff. Interestingly, you found a VERY high cutoff value. Crocombette used an ultrasolft pseudopotential I think, which yes does require a very high cutoff energy. I am not sure if you used a different pseudopotential than others, or if this pseudopotential is ultrasoft or PAW. Also, the valence of your pseudopotential is interesting… and not what I would expect. Perhaps this pseudopotential is trying to mimic localization effects by hybridizing the f and s orbitals. I don’t know.

Fitting the energy vs volume plot is a different way to do this determination of the bulk modulus, but yes, it is a valid way. However, the B-M EOS does not always accurately fit the data for solid state systems.

You state that “convergence of the calculations is higher.” I do not know what this means.

You did not extract a bulk modulus and only obtained data at a select number of U values. Also, I was looking for elastic constants, not just the bulk modulus. This requires individual directional strains.

This has the makings of achieving what I was looking for, but it did not quite get there.