Report on CuPd bcc to fcc transformation

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1 Neural work

A summary of the work performed on CuPd neural networking July 20-24th.

1.1 EOS of ground state configurations

A previous neural network performed revealed poor fits to ground state data produced from cluster expansions:

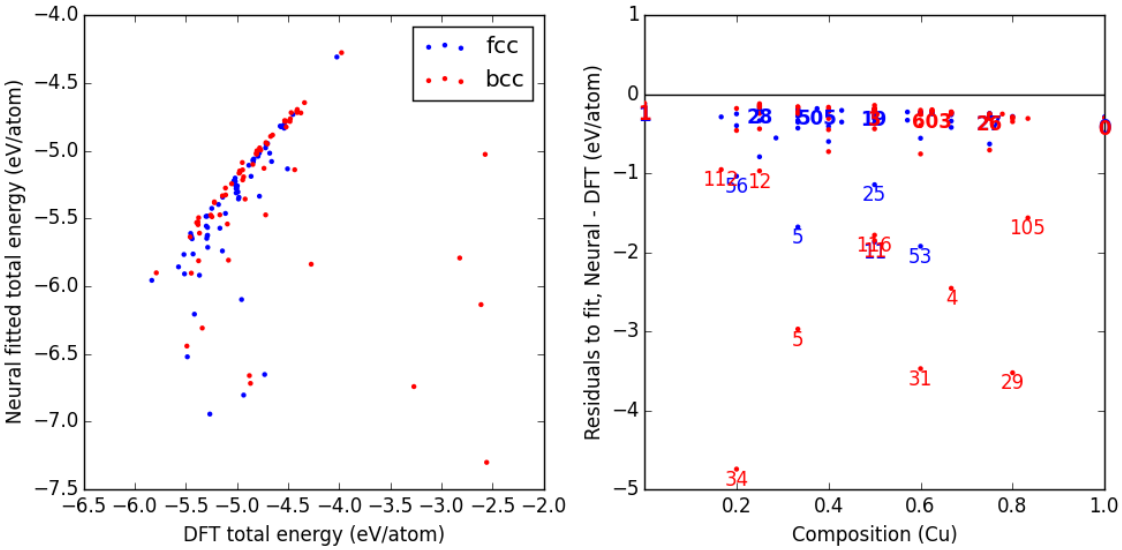
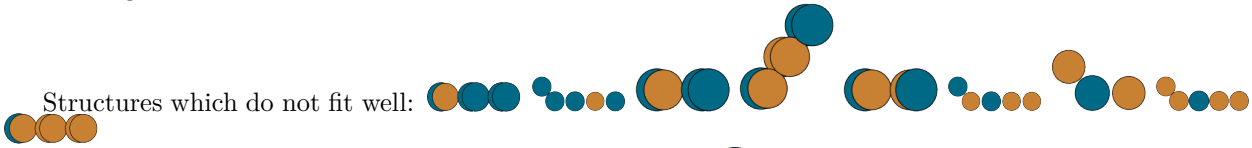


Figure 1: Residuals to initial NN fitting of GS energies for various CuPd structures from cluster expansion

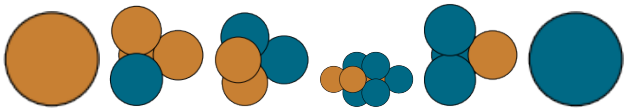
1.1.1 Problem structures

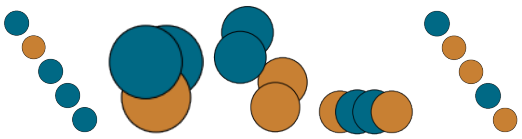
BCC configurations in fit:

Structures which do not fit well:



FCC configurations:



Structures which do not fit well: 

Visual inspection on the structures appears to show that "elongated" bulk configurations are likely to be candidates for poor prediction.

However, a more systematic approach is needed for identifying these poorly fitted regions.

One possible method of identifying dissimilar structures would be to use structure analysis tools. [?]

1.1.2 EOS of problematic structures

Further inspection revealed that the structures with the worst fits have very disordered EOS although nothing appears wrong with the geometries.

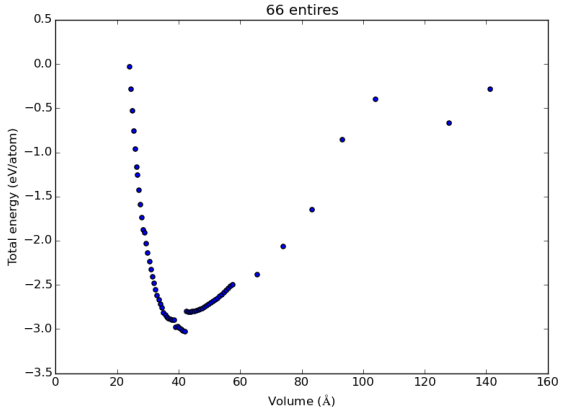


Figure 2: Equation of state for bcc configurations: 4, 5, 29, 31, and 34

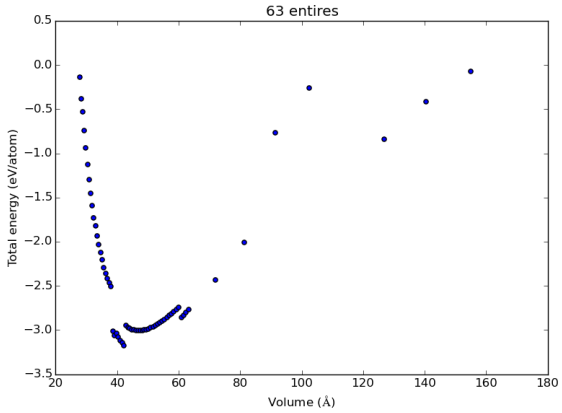


Figure 3: Equation of state for bcc configurations: 4, 5, 29, 31, and 34

There are some minor inconsistencies in certain fcc configurations as well.

The bcc structures shown above have been removed from all database moving forward.

I am not sure how to fix these calculations, or that it is worth the effort.

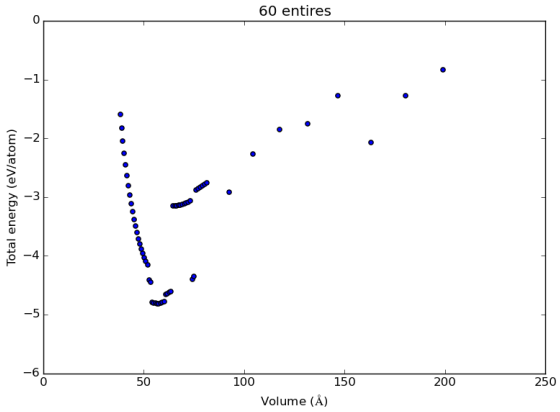


Figure 4: Equation of state for bcc configurations: 4, 5, 29, 31, and 34

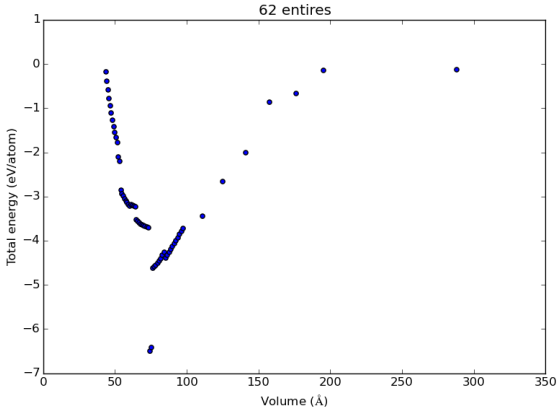


Figure 5: Equation of state for bcc configurations: 4, 5, 29, 31, and 34

1.2 Testing of multiple NNs

1.2.1 Fit to data included in NN

Initial NNs were trained with several structure types:

hiddenlayers: 2, 3, and 4 nodes: 30, 40, and 50

All residuals fit well to the data points included in the fitting process.

This suggests that it should be possible to produce highly accurate fits, even for alloys.

1.2.2 Fit to data NOT included in NN

The data at the end represents the bct structures included in the fitting and are magnified in Figure 13.

Again, very good (and rapid fitting) to all points of the PES for transition from fcc to bcc through bct configurations.

The mutliNN shows that surface predictions are not yet possible with the current model.

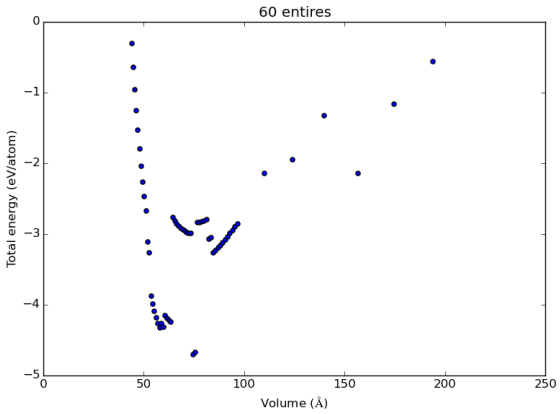


Figure 6: Equation of state for bcc configurations: 4, 5, 29, 31, and 34

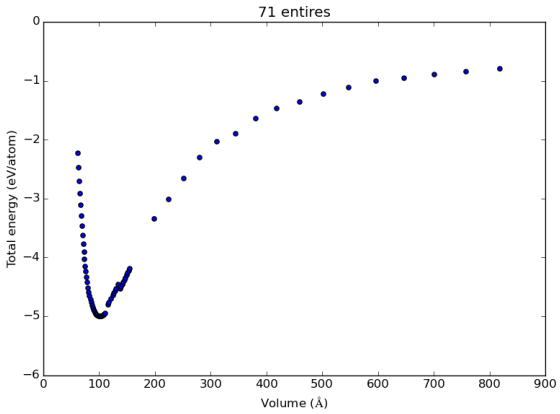


Figure 7: Equation of state for fcc configurations: 545, 548, and 552

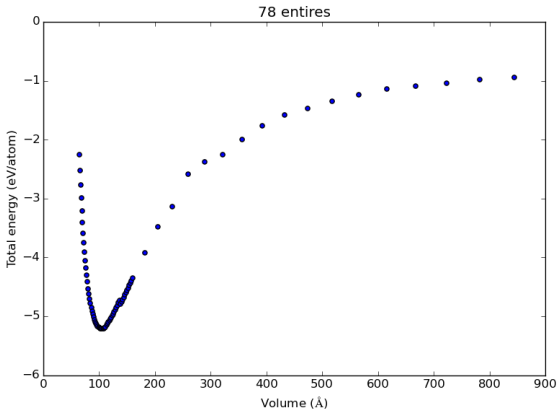


Figure 8: Equation of state for fcc configurations: 545, 548, and 552

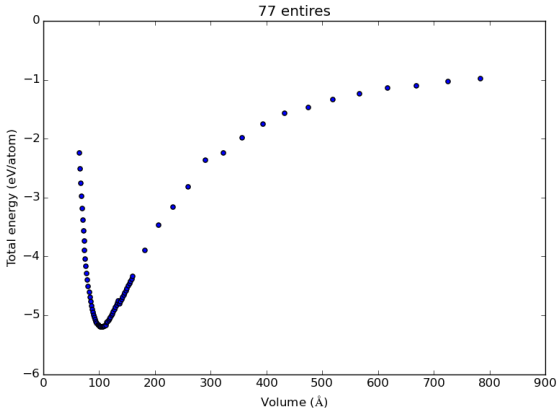


Figure 9: Equation of state for fcc configurations: 545, 548, and 552

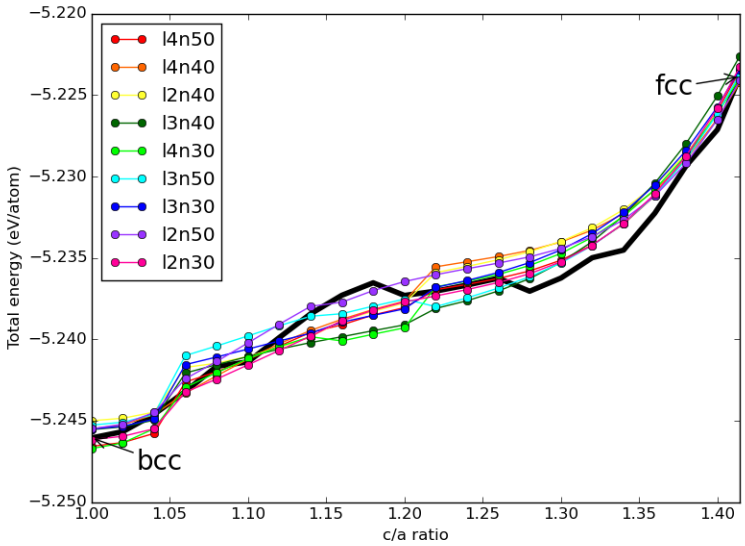


Figure 10: Neural network fit to fcc to bcc transition pathway (included in fitting data)

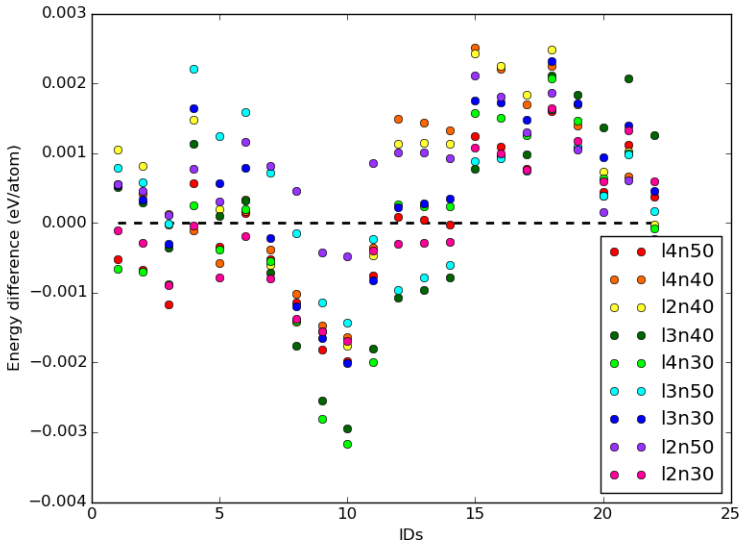


Figure 11: Residuals to above pathway data

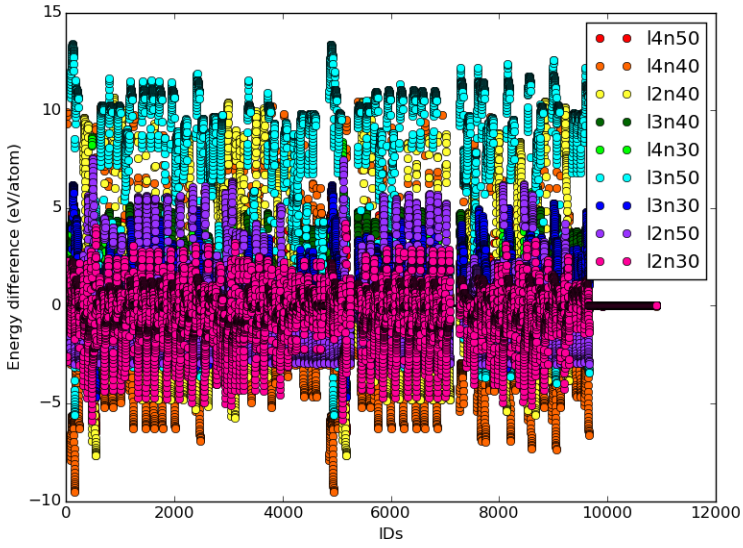


Figure 12: Residuals to all EOS in the database

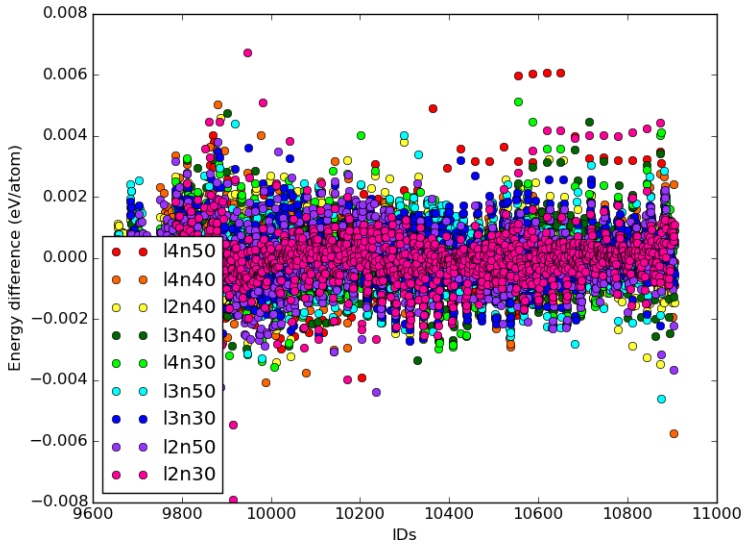


Figure 13: Residuals to bct data included in the fit

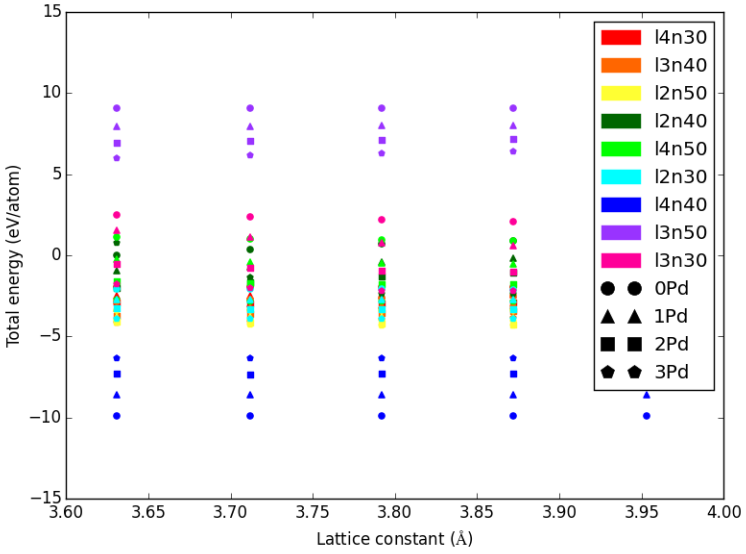


Figure 14: Multi-NN fit to various surface compositions of CuPd