PhD Log

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October 1, 2019

Contents

1 Tasks

1.1 TODO Ti3Al report—DFT chapter

- Start with the theory of DFT with the HK theorem and KS equations to solve for the density.
- Talk a bit about the approximations that are made.
- Alloy theory and the structure of Ti3Al
- Look at literature to do with all of this. Go through why solutes are incredibly important and why it is necessary do to this research.
- How can solutes lead to failure and why is oxygen in particular bad for the alloy.
- Is it wavy or planar slip
- Go into the calculations and what I have done for them
- Cite the research about the Fe and C vacancy concentration and what the implications are for alloy research
- What can I add to the research.

1.2 TODO Ti/Ti3Al DFT oxygen interstitial/vacancy binding energy

Want to find the vacancy formation energy, and the dissolution energy of oxygen interstitials at different sites in the Ti3Al lattice.

From these measurements we can then do a final calculation on the binding energy of oxygen to a vacancy thus elucidating if it is favourable comapared to just the normal positions.

This will provide insight into the high amount of vacancies with oxygen.

1.2.1 Notes on the calculations

1. Setting up relaxation

    - To set up one calculates the self consistent density first by not initiating

    relaxation.

    - Using the $\mathrm{OPTIONS}_{\mathrm{HF}}$ flag one can minimise the energy with respect to the

    Harris-Foulkes energy, which is far faster. And it would use the initial electron density for the relaxation, and then only calculate the density using the overlap of atomic densities.

    One is then able to minimise the energy accordingly.

2. Basis set optimisatons

    (a) Notes on the basis set It has been seen that the a smaller sphere radius for the oxygen was giving a much larger overlap (~17%) in the T2 interstitial site than any of the octahedral sites, which have an overlap of ~1.6%.

    This would have decreased the accuracy of the results.

    So to decrease the radius of the oxygen and to increase the completeness of the basis set one can introduce plane waves between certain energies such that the plane wave basis set is more complete.

    This should make the Harris-Foulkes energy smaller by the variational principle.

    <2019-05-23 Thu 18:19>

It seems that there is an optimal sphere radius of around 0.8. The best plane wave energy max seems to be at the maximum of around 3 Rydberg, but this is at the edge of the range of search so it seems that the range needs to be extended such that an optimum can be found before the basis set becomes overcomplete.

<2019-05-24 Fri 16:05>

There seems to be an optimum. I shall stop putting the plane wave basis set up in energy and now making pwemax = 4.0 ryd.

The best sphere radius for the oxygen is 0.78.

<2019-05-24 Fri 18:01>

Asking Dimitar about the plane wave basis set, he said to use the defaulf values that are generated when making a blm file.

(b) Perfect lattice spec name old rmax new rmax ratio 1 Ti 2.707297 3.024213 1.117060 2 Al 2.638772 2.947667 1.117060

Ti RSMH= 1.805 1.805 1.196 1.805 EH= -0.1 -0.1 -0.1 -0.1 RSMH2= 1.805 1.805 1.269 EH2= -0.9 -0.9 -0.9 P= 4.699 4.466 3.875 4.155 5.089 Al RSMH= 1.759 1.759 1.352 EH= -0.1 -0.1 -0.1 RSMH2= 1.759 1.759 EH2= -0.9 -0.9 P= 3.837 3.75 3.392 4.13 5.089

gmax = 6.6

Ti RSMH= 1.805 1.805 1.269 1.805 EH= -0.1 -0.1 -0.1 -0.1 RSMH2= 1.805 1.805 1.269 EH2= -0.9 -0.9 -0.9 P= 4.699 4.466 3.875 4.155 5.089 Al RSMH= 1.759 1.759 1.759 EH= -0.1 -0.1 -0.1 RSMH2= 1.759 1.759 EH2= -0.9 -0.9 P= 3.837 3.75 3.392 4.13 5.089

(c) O2 site (least overlap) spec name old rmax new rmax ratio 1 Ti 2.663548 2.746597 1.031179 2 Al 2.576718 2.746597 1.065928 3 O 1.662251 1.714079 1.031179

Ti RSMH= 1.776 1.776 1.254 1.776 EH= -0.1 -0.1 -0.1 -0.1 RSMH2= 1.776 1.776 1.254 EH2= -0.9 -0.9 -0.9 P= 4.686 4.447 3.874 4.155 5.089 PZ= 0 13.9381 Al RSMH= 1.718 1.718 1.718 EH= -0.1 -0.1 -0.1 RSMH2= 1.718 1.718 EH2= -0.9 -0.9 P= 3.83 3.74 3.389 4.13 5.089 O RSMH= 0.845 0.82 1.108 1.108 EH=-0.505 -0.1 -0.1 -0.1 RSMH2= 0.845 0.82 EH2= -1.305 -0.9 P= 2.886 2.858 3.25 4.11

(d) O1 site (next least overlap) spec name old rmax new rmax ratio 1 Ti 2.641151 2.734882 1.035489 2 Al 2.638731 3.547117 1.344251 3 O 1.666646 1.725793 1.035489

gmax = 9.8 Ti RSMH= 1.761 1.761 1.246 1.761 EH= -0.1 -0.1 -0.1 -0.1 RSMH2= 1.761 1.761 1.246 EH2= -0.9 -0.9 -0.9 P= 4.679 4.437 3.873 4.155 5.089 PZ= 0 13.9376 Al RSMH= 1.759 1.759

1.759 EH= -0.1 -0.1 -0.1 RSMH2= 1.759 1.759 EH2= -0.9 -0.9 P=3.837 3.75 3.392 4.13 5.089 O RSMH= 0.846 0.821 1.111 1.111 EH= -0.506 -0.1 -0.1 -0.1 RSMH2= 0.846 0.821 EH2= -1.306 -0.9 P= 2.886 2.859 3.25 4.11

(e) T1 site (next most overlap)

spec name old rmax new rmax ratio 1 Ti 2.654621 2.490980 0.938356 2 Al 2.586159 2.447921 0.946547 3 O 1.473639 1.382798 0.938356

gmax = 8.9

Ti RSMH= 1.77 1.77 1.251 1.77 EH= -0.1 -0.1 -0.1 -0.1 RSMH2= 1.77 1.77 1.251 EH2= -0.9 -0.9 -0.9 P= 4.683 4.443 3.874 4.155 5.089 PZ= 0 13.9379 Al RSMH=1.724 1.724 1.724 EH= -0.1 -0.1 -0.1 RSMH2= 1.724 1.724 EH2= -0.9 -0.9 P= 3.831 3.742 3.389 4.13 5.089 O RSMH= 0.831 0.982 0.982 0.982 EH= -0.474 -0.1 -0.1 -0.1 RSMH2= 0.831 0.982 EH2= -1.274 -0.9 P= 2.871 2.845 3.25 4.11

(f) T2 site (Most overlap)

1.2.2 Vacancy formation energy definition

$$ Δ $E_f^{vacancy}$ = $\lim_{N\{a\} \to \infty}$ \E(N{a}, 1)

- E(N{a} - 1, 0) \ $$

Where the first argument of the energy function is the number of lattice sites and the second denotes the number of vacancies. [1]

1.2.3 Dissoluton energy of species definition

The solution enthalpy of particular species is given by

$$E_{textsolution} = E(\mathrm{Ti}_N X_1) - E(\mathrm{Ti}_N) - E(X)$$

This is the same as a formation energy $\Delta E^{\mathrm{f}}_{\mathrm{O}}$

1.2.4 Vacancy-solute binding energy

[2]

$$ -E_{bind}(X - Vac) = E($Ti_{N - 2}$ X_1 Vac_1)

- E(Ti_N)
- E($Ti_{N - 1}$ X_1)

- E(Ti_{N-1} Vac_1) $$

where Vac is a vacancy, X is a solute impurity. The binding energy is negative here to keep with the convention that a *positive* binding energy is *favourable*.

I think that there really is a minus sign here
[3]
$$ $E_{bind}{}^{V - X} = +$ E(Ti_{N-1} X_1)

- E(Ti_{N-1} Vac_1)
- E(Ti_{N-2} X_1 Vac_1)
- E(Ti_N) $$

1.2.5 Dilute impurity energy and Vacancy formation energy

[2] $$ $E_{text\{impurity\}}(X) =$ E($Ti_{N-1}X_1$)

- N-1$\overline{NE(\mathrm{Ti_N})E(X)\$\$}$
  $$ $E_{text\{vacancy\}}(Vac) =$ E($Ti_{N-1}Vac_1$)
- N-1$\overline{NE(\mathrm{Ti_N})\$\$}$

1.2.6 Basis set

1.2.7 Relevant papers

[4]
[5]
[6]
[7]
[8]

Koizumi states that there is a preference for the interstitial site that is O1 (6 Ti atom coordination). O2 sites (4 Ti & 2 Al atom coordination), is of higher energy.

Site	Neighbouring atoms
O1	6 Ti
O2	4 Ti, 2 Al
T1	3 Ti, 1 Al (on Ti)
T2	3 Ti, 1 Al (on Al)

on Ti: the tetrahedral site is located just above a Ti atom in the c-axis direction. on Al: the tetrahedral site is located just above an Al atom in the c-axis direction.

$E_{vacancy formation}$

Author	Geometry	V_{Ti}	V_{Al}
Baulkin (2018)	2 x 2 x 2	2.209	2.894
Mishin (2000)	Embedded atom?	1.314	1.805

$E_{absorption}$ = - $E_{solution}$ The lower the solution the higher the binding energy the higher the absorption energy, the higher the binding energy.

Author	Geometry	O1	O2	T1	T2
Wei (2011)	Ti3Al/TiAl interface (6 & 6 layers)	6.23	4.75	4.20	3.83
Baulkin (2017)	2 x 2 x 2	6.16	4.69	4.24	3.78

During relaxation it was found that the tetrahedral sites are unstable and that they actually prefer the hexahedral sites (Baulkin).

The chemical potential/diatomic reference energy for the oxygen molecule decreases with increasing temperature.

T	(K)	0	500	1000	2000	2500	3000	4000	4500	5000
O	(eV)	4.35	4.89	5.5	6.83	7.54	8.27	9.78	10.55	11.34

[9]

Looked at point defects and soluted in an A_mB_n lattice.

It is difficult to determine the concentrations of both vacancies and antisite (substitutional of the other alloying element) defects reliably due to:

- Slow rates of diffusion -> Long equilibriation times.

Point-defect concentrations intimiately linked to chemical potentials of the constituents, and these chemical potentials can be used to discuss relative stability of different grain-boundary structures by comparing excess free energies.

We can say that there exists two sublattices, an A sublattice of m sites and a B sublattice of n sites, with all atoms of a particular type only belonging to that sublattice.

The alloy deviates slightly from stochiometry so we have A_xB_{1-x} where we suppose x to be within a few percent of $m/(m+n)$. Each site of each sublattice can by occupied by its own atom or an atom of the other kind or a vacancy.

c_{aa} = concentration of A atoms on the A sublattice; c_{bb} = concentration of B atoms on the B sublattice; c_{ab} = concentration of A atoms on the B sublattice; c_{ba} = concentration of B atoms on the A sublattice; c_{va} = concentration of vacancies on the A sublattice; c_{vb} = concentration of vacancies on the B sublattice.

Number of A and B sublattice cites are Nm and Nn. N is the number of fomulae units, which can vary due to the creation/annihilation of vacancies when the temperature or stochiometry varies, while the ratio m/n is constant.

A canonical ensemble is assumed so that the total numbers of A and B atoms are conserved.

There are 7 unknowns in a statistical model of the concentrations, c_i and N and they satisfy the constraints

$$c_{aa} + c_{ba} + c_{va} = 1$$

$$c_{bb} + c_{ab} + c_{vb} = 1$$

There are fixed numbers n_a and n_b of A and B atoms are given by

$$N(mc_{aa} + nc_{ab}) = n_a$$

$$N(mc_{ba} + nc_{bb}) = n_b$$

There are seven unknowns and four equations so there are three independent variables. The conservation of atoms constrains the possible defects which can be generated thermally. The effect of possible defect clustering or ordering is not included.

For a material of a single element, the calculation of, for example, the vacancy formation energy is simple: calculate the total energy of a perfect lattice and subtract it from the energy of a lattice with a defect. This is unique if N is sufficiently large and *the same number of atoms is compared* with and without the defect.

For an ordered alloy the stochiometry comes into account, so it is not as simple. The physical consequences, of having a working definition, are that we take the equilibrium concentrations of the four point defects and that they must be independent of the definition adoped for the point-defect energies, as long as the formulation is consistent.

If all we want at the end of the calcuation are the equilibrium point-defect concentrations, we do not need single point-defect energies, but rather the energies of threee independent stociometry-conserving complex defects. For example it is possible to compare the energy of a block AB containing a pair of vacancies or a triple defect with the energy of the same numbers of A and B atoms in a perfect crystal. However the above uniquely defined complex defect energies can be constructed simple from calculations of individual point-deect energies.

e_{mol}: Cohesive energy / energy per unit mole. We can arbitrariliy divide this between atoms of A and B type. This is a natural division in EAM potentials or BOP potentials which allocate energies to each atom.

$$e_{\mathrm{mol}} = me_{aa} + ne_{bb}$$

The energy of a block containing Nm sites of sublattice A and Nn sites of sublattice B is now:

\[E = Nm (c_{aa} e_{aa} + c_{ba} e_{ba} + c_{va} e_{va})

- Nn (c_{bb} e_{bb} + c_{ab} e_{ab} + c_{vb} e_{vb}) \]

The assumption has been made that the point defects are assumed to be sufficiently dilute that interactions may be neglected.

We can caw calculate the formation energy e_{vb} of a B vacancy. Construct block of N formula units with Nm sites of A, fully occupies by type A atoms, and $Nn - 1$ sites of type B with a vacancy on the remaining site.

$$e_{vb} = E(N, vb) - Nme_{aa} - (Nn - 1)e_{bb}$$

The energy of an A antisite is:

$$e_{ab} = E(N, ab) - Nme_{aa} - (Nn - 1)e_{bb}$$

One can define stochiometry-conserving complexes (in the case of NiAl)

$$e_{2v} = e_{va} + e_{vb}$$
$$e_{ta} = 2e_{vb} + e_{ba} - e_{bb}$$
$$e_{tb} = 2e_{va} + e_{ab} - e_{aa}$$

This formalism can be generalised to finite temperature if for *energy* we read *free energy* and the include both the vibrational entropy and the effect of temperature on the formation energies. (We are not including configurational entropy at this stage). Essentially one can do phonon calculations and then obtain the entropy from standard formulae. The effect is to add $-Ts_i$ to each of the e_i.

To find the enthalpy of the defected crystal, neglecting elastic strains, the total volume can be written as

\[V = Nm (c_{aa} Ω_{aa} + c_{ba} Ω_{ba} + c_{va} Ω_{va})

- Nn (c_{bb} Ω_{bb} + c_{ab} Ω_{ab} + c_{vb} Ω_{vb}) \]

where Ω_i are the partial molar volume and the quantity $m\Omega_{aa} + n\Omega_{bb}$ is uniquely defined as the volume per formula unit, but like the energies this is arbitrarily defined between A and B.

Relaxation volumes are uniquely defined, like that of a B vacancy:

$$\Omega_{bb} - \Omega_{vb} = N(m\Omega_{aa} + n\Omega_{bb}) - V(N, vb)$$

where $V(N, vb)$ is the volume of a crystal with N formula units with a single vacancy of the B sublattice.

Adding the pV term to construc the enthalpy amounts to replacing e_i by $e_i + p\Omega_i$ everywhere. The total Gibbs free energy without the configurational part is therefore given by replacing each of the e_i in the equations for e_{vb} and e_{ab} with $e_i + p\Omega_i - Ts_i$. These pressure and entropy terms are not included in the following for simplicity but they can be included.

The configurational entropy of the model system is

\[S = Nmk (c_{aa} log c_{aa} + c_{ba} log c_{ba} + c_{va} log c_{va})

- Nnk (c_{bb} log c_{bb} + c_{ab} log c_{ab} + c_{vb} log c_{vb}) \]

1.3 TODO Write up fitting and optimisation

- Used Genetic Algorithm and CMAES.
- Add in quantities to fit to.
- Realised that the prismatic fault was not high enough.

This caused incredibly large dissociation along the prismatic plane for a screw dislocation.

This was unreasonable, and it has been assumed that this can be rectified by a short ranged, very quickly decaying power law added to the pair potential.

Although this means that we need a refitting of the pair potential.

Unfortunately it seems that the accordance with the DFT results of the correct energetic ordering of the phases is lost: omega phase is **not** lower in energy than that of the hcp phase.

Reasonable starting point is:

PARAMETERS b2=60204900.7590034157 m2=-13.7544131202 p2=0.0000000000 fdd=0.2648249504 qdds=0.5697753882 qddp=0.5648597117 qddd=0.8213593849 b0=49.7557565400 p0=1.1050685730 b1=-5.097 3416100 p1=0.6991977165 ndt=2.0000000000 cr1=-6.0000000000 cr2=3.2217589360 r1dd=6.5000000000 rcdd=10.0000000000 cr3=-1.1418272350 rmaxhm=10.1000000000 npar=18 VARGS -vb2=60204900.7590034157 -vm2=-13.7544131202 -vp2=0.0000000000 -vfdd=0.2648249504 -vqdds=0.5697753882 -vqddp=0.5648597117 -vqddd=0.8213593849 -vb0=49.7557565400 -vp0=1. 1050685730 -vb1=-5.0973416100 -vp1=0.6991977165 -vndt=2.0000000000 -vcr1=-6.0000000000 -vcr2=3.2217589360 -vr1dd=6.5000000000 -vrcdd=10.0000000000 -vcr3=-1.1418272350 -vrma xhm=10.1000000000

Quantity predicted target $\mathrm{norm}_{\mathrm{pred}}$ $\mathrm{norm}_{\mathrm{tar}}$ sq diff. weight objective * 100^2

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a_{hcp} : 5.69823736 5.57678969 5.69823736 5.57678969 0.01474954 1000.00000000 147495.36 c/a : 1.57540221 1.58731122 15.29618259 15.41181168 0.01337009 100.00000000 13370.09 a_{omega} : 9.11713244 8.73254342 1.13964156 1.09156793 0.00231107 10.00000000 231.11 c_{omega} : 5.50357270 5.32343103 0.68794659 0.66542888 0.00050705 10.00000000 50.70 a_{4h} : 5.68949374 5.56325146 1.02269218 1.00000000 0.00051493 1.00000000 5.15 c_{4h} : 18.46292975 17.75908031 1.03963321 1.00000000 0.00157079 1.00000000 15.71 a_{6h} : 5.68593900 5.54639384 1.02515962 1.00000000 0.00063301 1.00000000 6.33 c_{6h} : 27.74967218 26.77136353 1.03654310 1.00000000 0.00133540 1.00000000 13.35 a_{bcc} : 6.20079768 6.17948863 0.88582824 0.88278409 0.00000927 1.00000000 0.09 a_{fcc} : 8.03310655 7.88677000 1.14758665 1.12668143 0.00043703 1.00000000 4.37 DE(o,h) : 1.19189500 -0.63343333 0.07945967 -0.04222889 0.01480810 3000.00000000 444243.14 DE(4h,h): 1.83337000 3.17160000 0.00733348 0.01268640 0.00002865 2000.00000000 573.08 DE(6h,h): 2.75695000 3.72005000 0.01102780 0.01488020 0.00001484 2000.00000000 296.82 DE(b,h) : 9.39020500 7.63520000 0.09485056 0.07712323 0.00031426 1.00000000 3.14 DE(f,h) : 4.17199500 4.51880000 0.04214136 0.04564444 0.00001227 2000.00000000 245.43 c_{11} : 211.10292175 176.10000000 0.92212869 0.76923077 0.02337778 100.00000000 23377.78 c_{33} : 232.93926611 190.50000000 0.94059869 0.76923077 0.02936697 100.00000000 29366.97 c_{44} : 55.49057353 50.80000000 0.84025702 0.76923077 0.00504473 100.00000000 5044.73 c_{12} : 110.56430372 86.90000000 0.97870500 0.76923077 0.04387945 100.00000000 43879.45 c_{13} : 73.53441848 68.30000000 0.82818356 0.76923077 0.00347543 10.00000000 347.54 M_{freq0}: 2.86541811 2.85858719 0.20883117 0.20833333 0.00000025 0.10000000 0.00 M_{freq1}: 2.86541812 2.85858719 0.20883117 0.20833333 0.00000025 0.10000000 0.00 M_{freq2}: 2.86541812 2.85858719 0.20883117 0.20833333 0.00000025 0.10000000 0.00 M_{freq3}: 2.86541813 2.85858719 0.20883117 0.20833333 0.00000025 0.10000000 0.00 M_{freq4}: 6.16074486 5.66706047 0.22648223 0.20833333 0.00032938 0.10000000 0.33 M_{freq5}: 6.16074486 5.66706047 0.22648223 0.20833333 0.00032938 0.10000000 0.33 H_{freq0}: 4.29880135 4.80643423 0.18633015 0.20833333 0.00048414 0.10000000 0.48 H_{freq1}: 4.29880135 5.58010025 0.16049597 0.20833333 0.00228841

0.10000000 2.29 H_{freq2}: 6.76073943 5.65316738 0.24915013 0.20833333 0.00166601 0.10000000 1.67 H_{freq3}: 6.76073943 6.36651842 0.22123354 0.20833333 0.00016642 0.10000000 0.17 H_{freq4}: 8.32761036 6.40050186 0.27105981 0.20833333 0.00393461 0.10000000 3.93 H_{freq5}: 8.32761036 7.64082373 0.22705913 0.20833333 0.00035066 0.10000000 0.35 bandw. G: 4.58784139 5.87085872 1.30243337 1.66666667 0.13266589 15.00000000 19899.88 bandw. K: 5.68718179 4.97424321 1.03938731 0.90909091 0.01697715 15.00000000 2546.57 bandw. M: 6.52257165 7.78109872 1.39709740 1.66666667 0.07266759 15.00000000 10900.14 bandw. L: 5.25996287 6.34433701 1.38179999 1.66666667 0.08114903 15.00000000 12172.35 bandw. H: 4.39872218 9.70902614 0.41186812 0.90909091 0.24723050 5.00000000 12361.53 $DOSerr_h$: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000 0.00 $DOSerr_o$: 95.30342229 0.00000000 95.30342229 0.00000000 9082.74230017 0.00000000 0.00 E_{prisf}: 119.59113352 220.00000000 119.59113352 220.00000000 10081.94046857 100000.00000000 10081940468565.85

PARAMETERS b2=73362700.7877650857 m2=-13.9508390550 p2=0.0000000000 fdd=0.2648249504 qdds=0.5697753882 qddp=0.5648597117 qddd=0.8213593849 b0=49.7557565400 p0=1.1050685730 b1=-5.097 3416100 p1=0.6991977165 ndt=2.0000000000 cr1=-6.0000000000 cr2=3.2217589360 r1dd=6.5000000000 rcdd=10.0000000000 cr3=-1.1418272350 rmaxhm=10.1000000000 npar=18 VARGS -vb2=73362700.7877650857 -vm2=-13.9508390550 -vp2=0.0000000000 -vfdd=0.2648249504 -vqdds=0.5697753882 -vqddp=0.5648597117 -vqddd=0.8213593849 -vb0=49.7557565400 -vp0=1. 1050685730 -vb1=-5.0973416100 -vp1=0.6991977165 -vndt=2.0000000000 -vcr1=-6.0000000000 -vcr2=3.2217589360 -vr1dd=6.5000000000 -vrcdd=10.0000000000 -vcr3=-1.1418272350 -vrma xhm=10.1000000000

Quantity predicted target $norm_{pred}$ $norm_{tar}$ sq diff. weight objective * 100^2

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a_{hcp} : 5.68326063 5.57678969 5.68326063 5.57678969 0.01133606 1000.00000000 113360.60 c/a : 1.58164523 1.58731122 15.35679851 15.41181168 0.00302645 100.00000000 3026.45 a_{omega} : 9.09093887 8.73254342 1.13636736 1.09156793 0.00200699 10.00000000 200.70 c_{omega} : 5.49075443 5.32343103 0.68634430 0.66542888 0.00043745 10.00000000 43.75 a_{4h} : 5.67495771 5.56325146 1.02007931 1.00000000 0.00040318 1.00000000 4.03 c_{4h} : 18.41194892 17.75908031 1.03676252 1.00000000 0.00135148 1.00000000 13.51 a_{6h} : 5.67118026 5.54639384 1.02249866 1.00000000 0.00050619 1.00000000 5.06 c_{6h} : 27.67479817 26.77136353 1.03374631 1.00000000 0.00113881 1.00000000 11.39 a_{bcc} : 6.20079768 6.17948863 0.88582824 0.88278409 0.00000927 1.00000000 0.09 a_{fcc} : 8.01192626 7.88677000 1.14456089 1.12668143 0.00031968 1.00000000 3.20 DE(o,h) : 1.09675833 -0.63343333 0.07311722 -0.04222889 0.01330473 3000.00000000 399141.76 DE(4h,h): 1.84836500 3.17160000 0.00739346 0.01268640 0.00002802 2000.00000000 560.30 DE(6h,h):

2.77866667 3.72005000 0.01111467 0.01488020 0.00001418 2000.00000000 283.58 DE(b,h) : 8.85897500 7.63520000 0.08948460 0.07712323 0.00015280 1.00000000 1.53 DE(f,h) : 4.20064500 4.51880000 0.04243076 0.04564444 0.00001033 2000.00000000 206.56 c_{11} : 209.98522208 176.10000000 0.91724642 0.76923077 0.02190863 100.00000000 21908.63 c_{33} : 232.98310764 190.50000000 0.94077572 0.76923077 0.02942767 100.00000000 29427.67 c_{44} : 54.68686450 50.80000000 0.82808699 0.76923077 0.00346405 100.00000000 3464.05 c_{12} : 109.06955946 86.90000000 0.96547366 0.76923077 0.03851127 100.00000000 38511.27 c_{13} : 73.74195452 68.30000000 0.83052094 0.76923077 0.00375649 10.00000000 375.65 M_{freq0}: 2.85519402 2.85858719 0.20808604 0.20833333 0.00000006 0.10000000 0.00 M_{freq1}: 2.85519403 2.85858719 0.20808604 0.20833333 0.00000006 0.10000000 0.00 M_{freq2}: 2.85519403 2.85858719 0.20808604 0.20833333 0.00000006 0.10000000 0.00 M_{freq3}: 2.85519404 2.85858719 0.20808604 0.20833333 0.00000006 0.10000000 0.00 M_{freq4}: 6.14081288 5.66706047 0.22574949 0.20833333 0.00030332 0.10000000 0.30 M_{freq5}: 6.14081288 5.66706047 0.22574949 0.20833333 0.00030332 0.10000000 0.30 H_{freq0}: 4.24870561 4.80643423 0.18415877 0.20833333 0.00058441 0.10000000 0.58 H_{freq1}: 4.24870561 5.58010025 0.15862565 0.20833333 0.00247085 0.10000000 2.47 H_{freq2}: 6.73808691 5.65316738 0.24831533 0.20833333 0.00159856 0.10000000 1.60 H_{freq3}: 6.73808691 6.36651842 0.22049227 0.20833333 0.00014784 0.10000000 0.15 H_{freq4}: 8.32193375 6.40050186 0.27087504 0.20833333 0.00391147 0.10000000 3.91 H_{freq5}: 8.32193375 7.64082373 0.22690436 0.20833333 0.00034488 0.10000000 0.34 bandw. G: 4.63954304 5.87085872 1.31711085 1.66666667 0.12218927 15.00000000 18328.39 bandw. K: 5.74840743 4.97424321 1.05057689 0.90909091 0.02001828 15.00000000 3002.74 bandw. M: 6.57699445 7.78109872 1.40875444 1.66666667 0.06651871 15.00000000 9977.81 bandw. L: 5.31166452 6.34433701 1.39538209 1.66666667 0.07359532 15.00000000 11039.30 bandw. H: 4.44226042 9.70902614 0.41594476 0.90909091 0.24319312 5.00000000 12159.66 $DOSerr_h$: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000 0.00 $DOSerr_o$: 98.57124703 0.00000000 98.57124703 0.00000000 9716.29074056 0.00000000 0.00 E_{prisf}: 119.88060210 220.00000000 119.88060210 220.00000000 10023.89383558 100000.00000000 10023893835581.32

b2=91394018.8920019716 m2=-14.4689417704 p2=0.0000000000 fdd=0.2648249504 qdds=0.5697753882 qddp=0.5648597117 qddd=0.8213593849 b0=49.7557565400 p0=1.1050685730 b1=-5.097 3416100 p1=0.6991977165 ndt=2.0000000000 cr1=-6.0000000000 cr2=3.2217589360 r1dd=6.5000000000 rcdd=10.0000000000 cr3=-1.1418272350 rmaxhm=10.1000000000 npar=18 VARGS -vb2=91394018.8920019716 -vm2=-14.4689417704 -vp2=0.0000000000 -vfdd=0.2648249504 -vqdds=0.5697753882 -vqddp=0.5648597117 -vqddd=0.8213593849 -vb0=49.7557565400 -vp0=1. 1050685730 -vb1=-5.0973416100 -vp1=0.6991977165 -vndt=2.0000000000 - vcr1=-6.0000000000 -vcr2=3.2217589360 -vr1dd=6.5000000000 -vrcdd=10.0000000000

-vcr3=-1.1418272350 -vrma xhm=10.1000000000

Quantity predicted target $norm_{pred}$ $norm_{tar}$ sq diff. weight objective * 100^2

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a_{hcp} : 5.62525983 5.57678969 5.62525983 5.57678969 0.00234935 1000.00000000 23493.55 c/a : 1.60613643 1.58731122 15.59459288 15.41181168 0.03340896 100.00000000 33408.96 a_{omega} : 8.98530887 8.73254342 1.12316361 1.09156793 0.00099829 10.00000000 99.83 c_{omega} : 5.44549052 5.32343103 0.68068632 0.66542888 0.00023279 10.00000000 23.28 a_{4h} : 5.61807095 5.56325146 1.00985386 1.00000000 0.00009710 1.00000000 0.97 c_{4h} : 18.21768083 17.75908031 1.02582344 1.00000000 0.00066685 1.00000000 6.67 a_{6h} : 5.61365761 5.54639384 1.01212748 1.00000000 0.00014708 1.00000000 1.47 c_{6h} : 27.38802263 26.77136353 1.02303428 1.00000000 0.00053058 1.00000000 5.31 a_{bcc} : 6.20079768 6.17948863 0.88582824 0.88278409 0.00000927 1.00000000 0.09 a_{fcc} : 7.93028587 7.88677000 1.13289798 1.12668143 0.00003865 1.00000000 0.39 DE(o,h) : 0.56552167 -0.63343333 0.03770144 -0.04222889 0.00638886 3000.00000000 191665.75 DE(4h,h): 1.90610750 3.17160000 0.00762443 0.01268640 0.00002562 2000.00000000 512.47 DE(6h,h): 2.86158833 3.72005000 0.01144635 0.01488020 0.00001179 2000.00000000 235.83 DE(b,h) : 7.52522500 7.63520000 0.07601237 0.07712323 0.00000123 1.00000000 0.01 DE(f,h) : 4.31089500 4.51880000 0.04354439 0.04564444 0.00000441 2000.00000000 88.20 c_{11} : 199.90553801 176.10000000 0.87321687 0.76923077 0.01081311 100.00000000 10813.11 c_{33} : 226.98933014 190.50000000 0.91657311 0.76923077 0.02170976 100.00000000 21709.76 c_{44} : 52.69685443 50.80000000 0.79795358 0.76923077 0.00082500 100.00000000 825.00 c_{12} : 98.48673287 86.90000000 0.87179546 0.76923077 0.01051952 100.00000000 10519.52 c_{13} : 72.19938307 68.30000000 0.81314769 0.76923077 0.00192870 10.00000000 192.87 M_{freq0}: 2.78990046 2.85858719 0.20332746 0.20833333 0.00002506 0.10000000 0.03 M_{freq1}: 2.78990047 2.85858719 0.20332746 0.20833333 0.00002506 0.10000000 0.03 M_{freq2}: 2.78990047 2.85858719 0.20332746 0.20833333 0.00002506 0.10000000 0.03 M_{freq3}: 2.78990048 2.85858719 0.20332746 0.20833333 0.00002506 0.10000000 0.03 M_{freq4}: 6.00974100 5.66706047 0.22093101 0.20833333 0.00015870 0.10000000 0.16 M_{freq5}: 6.00974100 5.66706047 0.22093101 0.20833333 0.00015870 0.10000000 0.16 H_{freq0}: 3.99826489 4.80643423 0.17330350 0.20833333 0.00122709 0.10000000 1.23 H_{freq1}: 3.99826489 5.58010025 0.14927543 0.20833333 0.00348784 0.10000000 3.49 H_{freq2}: 6.58970446 5.65316738 0.24284706 0.20833333 0.00119120 0.10000000 1.19 H_{freq3}: 6.58970446 6.36651842 0.21563671 0.20833333 0.00005334 0.10000000 0.05 H_{freq4}: 8.23482251 6.40050186 0.26803961 0.20833333 0.00356484 0.10000000 3.56 H_{freq5}: 8.23482251 7.64082373 0.22452920 0.20833333 0.00026231 0.10000000 0.26 bandw. G: 4.85043136 5.87085872 1.37697953 1.66666667 0.08391864 15.00000000 12587.80 bandw. K: 5.99194943 4.97424321 1.09508653

0.90909091 0.03459437 15.00000000 5189.16 bandw. M: 6.79332504 7.78109872 1.45509122 1.66666667 0.04476417 15.00000000 6714.63 bandw. L: 5.51847114 6.34433701 1.44971049 1.66666667 0.04706998 15.00000000 7060.50 bandw. H: 4.61097107 9.70902614 0.43174174 0.90909091 0.22786222 5.00000000 11393.11 $\mathrm{DOSerr_h}$: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000 0.00 $\mathrm{DOSerr_o}$: 111.68287062 0.00000000 111.68287062 0.00000000 12473.06358905 0.00000000 0.00 $\mathrm{E_{prisf}}$: 105.39637060 220.00000000 105.39637060 220.00000000 13133.99187172 100000.00000000 13133991871718.04

PARAMETERS b2=901772799.4098891020 m2=-15.7042290440 p2=0.0000000000 fdd=0.2648249504 qdds=0.5697753882 qddp=0.5648597117 qddd=0.8213593849 b0=47.9215925588 p0=1.1092837121 b1=-3.99 59790920 p1=0.6574344463 ndt=2.0000000000 cr1=-6.0000000000 cr2=3.2217589360 r1dd=6.5000000000 rcdd=10.0000000000 cr3=-1.1418272350 rmaxhm=10.1000000000 npar=18 VARGS -vb2=901772799.4098891020 -vm2=-15.7042290440 -vp2=0.0000000000 -vfdd=0.2648249504 -vqdds=0.5697753882 -vqddp=0.5648597117 -vqddd=0.8213593849 -vb0=47.9215925588 -vp0=1 .1092837121 -vb1=-3.9959790920 -vp1=0.6574344463 -vndt=2.0000000000 -vcr1=-6.0000000000 -vcr2=3.2217589360 -vr1dd=6.5000000000 -vrcdd=10.0000000000 -vcr3=-1.1418272350 -vrm axhm=10.1000000000

Quantity predicted target $\mathrm{norm_{pred}}$ $\mathrm{norm_{tar}}$ sq diff. weight objective * 100^2

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a_{hcp} : 5.58632034 5.57678969 5.58632034 5.57678969 0.00009083 1000.00000000 908.33 c/a : 1.58324912 1.58731122 15.37237127 15.41181168 0.00155555 100.00000000 1555.55 a_{omega} : 8.94268260 8.73254342 1.11783533 1.09156793 0.00068998 10.00000000 69.00 c_{omega} : 5.41189311 5.32343103 0.67648664 0.66542888 0.00012227 10.00000000 12.23 a_{4h} : 5.57986672 5.56325146 1.00298661 1.00000000 0.00000892 1.00000000 0.09 c_{4h} : 18.08926296 17.75908031 1.01859233 1.00000000 0.00034567 1.00000000 3.46 a_{6h} : 5.57525690 5.54639384 1.00520393 1.00000000 0.00002708 1.00000000 0.27 c_{6h} : 27.19488908 26.77136353 1.01582010 1.00000000 0.00025028 1.00000000 2.50 a_{bcc} : 6.20079768 6.17948863 0.88582824 0.88278409 0.00000927 1.00000000 0.09 a_{fcc} : 7.87598731 7.88677000 1.12514104 1.12668143 0.00000237 1.00000000 0.02 DE(o,h) : 1.34781000 -0.63343333 0.08985400 -0.04222889 0.01744589 3000.00000000 523376.69 DE(4h,h): 2.01890750 3.17160000 0.00807563 0.01268640 0.00002126 2000.00000000 425.18 DE(6h,h): 3.01372500 3.72005000 0.01205490 0.01488020 0.00000798 2000.00000000 159.65 DE(b,h) : 7.98701000 7.63520000 0.08067687 0.07712323 0.00001263 1.00000000 0.13 DE(f,h) : 4.52676000 4.51880000 0.04572485 0.04564444 0.00000001 2000.00000000 0.13 c_{11} : 221.16376396 176.10000000 0.96607594 0.76923077 0.03874802 100.00000000 38748.02 c_{33} : 262.04112894 190.50000000 1.05811076 0.76923077 0.08345165 100.00000000 83451.65 c_{44} : 61.54190626 50.80000000

0.93188834 0.76923077 0.02645749 100.00000000 26457.49 c_{12} : 103.69257328 86.90000000 0.91787708 0.76923077 0.02209572 100.00000000 22095.72 c_{13} : 80.66574593 68.30000000 0.90850035 0.76923077 0.01939602 10.00000000 1939.60 M_{freq0}: 3.01657581 2.85858719 0.21984752 0.20833333 0.00013258 0.10000000 0.13 M_{freq1}: 3.01657582 2.85858719 0.21984752 0.20833333 0.00013258 0.10000000 0.13 M_{freq2}: 3.01657582 2.85858719 0.21984752 0.20833333 0.00013258 0.10000000 0.13 M_{freq3}: 3.01657583 2.85858719 0.21984752 0.20833333 0.00013258 0.10000000 0.13 M_{freq4}: 6.55202353 5.66706047 0.24086648 0.20833333 0.00105841 0.10000000 1.06 M_{freq5}: 6.55202353 5.66706047 0.24086648 0.20833333 0.00105841 0.10000000 1.06 H_{freq0}: 4.22631935 4.80643423 0.18318844 0.20833333 0.00063227 0.10000000 0.63 H_{freq1}: 4.22631935 5.58010025 0.15778985 0.20833333 0.00255464 0.10000000 2.55 H_{freq2}: 7.21414462 5.65316738 0.26585924 0.20833333 0.00330923 0.10000000 3.31 H_{freq3}: 7.21414462 6.36651842 0.23607044 0.20833333 0.00076935 0.10000000 0.77 H_{freq4}: 8.98961736 6.40050186 0.29260783 0.20833333 0.00710219 0.10000000 7.10 H_{freq5}: 8.98961736 7.64082373 0.24510930 0.20833333 0.00135247 0.10000000 1.35 bandw. G: 4.99873347 5.87085872 1.41908073 1.66666667 0.06129880 15.00000000 9194.82 bandw. K: 6.15929951 4.97424321 1.12567138 0.90909091 0.04690710 15.00000000 7036.06 bandw. M: 6.94162715 7.78109872 1.48685668 1.66666667 0.03233163 15.00000000 4849.74 bandw. L: 5.69262407 6.34433701 1.49546072 1.66666667 0.02931148 15.00000000 4396.72 bandw. H: 4.72525894 9.70902614 0.44244293 0.90909091 0.21776034 5.00000000 10888.02 $DOSerr_h$: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000 0.00 $DOSerr_o$: 93.81903067 0.00000000 93.81903067 0.00000000 8802.01051603 0.00000000 0.00 E_{prisf}: 121.13361833 220.00000000 121.13361833 220.00000000 9774.56142366 1.00000000 97745614.24

PARAMETERS b2=999299811.2360876799 m2=-15.0812332826 p2=0.0000000000 fdd=0.2648249504 qdds=0.5697753882 qddp=0.5648597117 qddd=0.8213593849 b0=47.4028718523 p0=1.1110171622 b1=-4.02 76308878 p1=0.6595005412 ndt=2.0000000000 cr1=-6.0000000000 cr2=3.2217589360 r1dd=6.5000000000 rcdd=10.0000000000 cr3=-1.1418272350 rmaxhm=10.1000000000 npar=18 VARGS -vb2=999299811.2360876799 -vm2=-15.0812332826 -vp2=0.0000000000 -vfdd=0.2648249504 -vqdds=0.5697753882 -vqddp=0.5648597117 -vqddd=0.8213593849 -vb0=47.4028718523 -vp0=1 .1110171622 -vb1=-4.0276308878 -vp1=0.6595005412 -vndt=2.0000000000 -vcr1=-6.0000000000 -vcr2=3.2217589360 -vr1dd=6.5000000000 -vrcdd=10.0000000000 -vcr3=-1.1418272350 -vrm axhm=10.1000000000

Quantity predicted target $norm_{pred}$ $norm_{tar}$ sq diff. weight objective * 100^2

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a_{hcp} : 5.70613418 5.57678969 5.70613418 5.57678969 0.01673000 1000.00000000 167299.96 c/a : 1.57212363 1.58731122 15.26434959 15.41181168 0.02174507

100.00000000 21745.07 a_{omega} : 9.16691334 8.73254342 1.14586417 1.09156793 0.00294808 10.00000000 294.81 c_{omega} : 5.50859785 5.32343103 0.68857473 0.66542888 0.00053573 10.00000000 53.57 a_{4h} : 5.69646904 5.56325146 1.02394599 1.00000000 0.00057341 1.00000000 5.73 c_{4h} : 18.49515166 17.75908031 1.04144761 1.00000000 0.00171790 1.00000000 17.18 a_{6h} : 5.69332284 5.54639384 1.02649091 1.00000000 0.00070177 1.00000000 7.02 c_{6h} : 27.79206990 26.77136353 1.03812680 1.00000000 0.00145365 1.00000000 14.54 a_{bcc} : 6.20079768 6.17948863 0.88582824 0.88278409 0.00000927 1.00000000 0.09 a_{fcc} : 8.04427434 7.88677000 1.14918205 1.12668143 0.00050628 1.00000000 5.06 DE(o,h) : 3.32247167 -0.63343333 0.22149811 -0.04222889 0.06955193 3000.00000000 2086557.92 DE(4h,h): 1.86745000 3.17160000 0.00746980 0.01268640 0.00002721 2000.00000000 544.26 DE(6h,h): 2.80055333 3.72005000 0.01120221 0.01488020 0.00001353 2000.00000000 270.55 DE(b,h) : 11.65659500 7.63520000 0.11774338 0.07712323 0.00165000 1.00000000 16.50 DE(f,h) : 4.23754500 4.51880000 0.04280348 0.04564444 0.00000807 2000.00000000 161.42 c_{11} : 256.25825401 176.10000000 1.11937384 0.76923077 0.12260017 100.00000000 122600.17 c_{33} : 285.11928542 190.50000000 1.15129936 0.76923077 0.14597640 100.00000000 145976.40 c_{44} : 69.13492938 50.80000000 1.04686447 0.76923077 0.07708047 100.00000000 77080.47 c_{12} : 132.18803667 86.90000000 1.17011628 0.76923077 0.16070920 100.00000000 160709.20 c_{13} : 85.78433896 68.30000000 0.96614865 0.76923077 0.03877665 10.00000000 3877.67 M_{freq0}: 3.29251267 2.85858719 0.23995775 0.20833333 0.00100010 0.10000000 1.00 M_{freq1}: 3.29251269 2.85858719 0.23995775 0.20833333 0.00100010 0.10000000 1.00 M_{freq2}: 3.29251269 2.85858719 0.23995775 0.20833333 0.00100010 0.10000000 1.00 M_{freq3}: 3.29251270 2.85858719 0.23995775 0.20833333 0.00100010 0.10000000 1.00 M_{freq4}: 7.05767677 5.66706047 0.25945538 0.20833333 0.00261346 0.10000000 2.61 M_{freq5}: 7.05767677 5.66706047 0.25945538 0.20833333 0.00261346 0.10000000 2.61 H_{freq0}: 4.96582422 4.80643423 0.21524204 0.20833333 0.00004773 0.10000000 0.05 H_{freq1}: 4.96582422 5.58010025 0.18539931 0.20833333 0.00052597 0.10000000 0.53 H_{freq2}: 7.78709460 5.65316738 0.28697388 0.20833333 0.00618434 0.10000000 6.18 H_{freq3}: 7.78709460 6.36651842 0.25481924 0.20833333 0.00216094 0.10000000 2.16 H_{freq4}: 9.46161176 6.40050186 0.30797102 0.20833333 0.00992767 0.10000000 9.93 H_{freq5}: 9.46161176 7.64082373 0.25797861 0.20833333 0.00246465 0.10000000 2.46 bandw. G: 4.56062999 5.87085872 1.29470838 1.66666667 0.13835297 15.00000000 20752.94 bandw. K: 5.65452812 4.97424321 1.03341954 0.90909091 0.01545761 15.00000000 2318.64 bandw. M: 6.49399969 7.78109872 1.39097744 1.66666667 0.07600455 15.00000000 11400.68 bandw. L: 5.23275148 6.34433701 1.37465151 1.66666667 0.08527285 15.00000000 12790.93 bandw. H: 4.37695307 9.70902614 0.40982980 0.90909091 0.24926165 5.00000000 12463.08 $DOSerr_h$: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000 0.00 $DOSerr_o$: 79.18263924 0.00000000 79.18263924 0.00000000 6269.89035742

0.00000000 0.00 E_{prisf}: 216.93072664 220.00000000 216.93072664 220.00000000 9.42043896 0.01000000 942.04

PARAMETERS b2=883425978.8605744839 m2=-15.9116989631 p2=0.0000000000 fdd=0.2648249504 qdds=0.5697753882 qddp=0.5648597117 qddd=0.8213593849 b0=48.9271746890 p0=1.1172295299 b1=-3.80 34356258 p1=0.6525724680 ndt=2.0000000000 cr1=-6.0000000000 cr2=3.2217589360 r1dd=6.5000000000 rcdd=10.0000000000 cr3=-1.1418272350 rmaxhm=10.1000000000 npar=18 VARGS -vb2=883425978.8605744839 -vm2=-15.9116989631 -vp2=0.0000000000 -vfdd=0.2648249504 -vqdds=0.5697753882 -vqddp=0.5648597117 -vqddd=0.8213593849 -vb0=48.9271746890 -vp0=1 .1172295299 -vb1=-3.8034356258 -vp1=0.6525724680 -vndt=2.0000000000 -vcr1=-6.0000000000 -vcr2=3.2217589360 -vr1dd=6.5000000000 -vrcdd=10.0000000000 -vcr3=-1.1418272350 -vrm axhm=10.1000000000

Quantity predicted target $norm_{pred}$ $norm_{tar}$ sq diff. weight objective * 100^2

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a_{hcp} : 5.55915799 5.57678969 5.55915799 5.57678969 0.00031088 1000.00000000 3108.77 c/a : 1.59486281 1.58731122 15.48513296 15.41181168 0.00537601 100.00000000 5376.01 a_{omega} : 8.89176293 8.73254342 1.11147037 1.09156793 0.00039611 10.00000000 39.61 c_{omega} : 5.39115562 5.32343103 0.67389445 0.66542888 0.00007167 10.00000000 7.17 a_{4h} : 5.55256003 5.56325146 0.99807820 1.00000000 0.00000369 1.00000000 0.04 c_{4h} : 17.99793925 17.75908031 1.01344996 1.00000000 0.00018090 1.00000000 1.81 a_{6h} : 5.54765195 5.54639384 1.00022683 1.00000000 0.00000005 1.00000000 0.00 c_{6h} : 27.05991164 26.77136353 1.01077824 1.00000000 0.00011617 1.00000000 1.16 a_{bcc} : 6.20079768 6.17948863 0.88582824 0.88278409 0.00000927 1.00000000 0.09 a_{fcc} : 7.83651495 7.88677000 1.11950214 1.12668143 0.00005154 1.00000000 0.52 DE(o,h) : 1.00654333 -0.63343333 0.06710289 -0.04222889 0.01195344 3000.00000000 358603.13 DE(4h,h): 2.04859250 3.17160000 0.00819437 0.01268640 0.00002018 2000.00000000 403.57 DE(6h,h): 3.05533667 3.72005000 0.01222135 0.01488020 0.00000707 2000.00000000 141.39 DE(b,h) : 8.01955000 7.63520000 0.08100556 0.07712323 0.00001507 1.00000000 0.15 DE(f,h) : 4.58537000 4.51880000 0.04631687 0.04564444 0.00000045 2000.00000000 9.04 c_{11} : 214.45221283 176.10000000 0.93675889 0.76923077 0.02806567 100.00000000 28065.67 c_{33} : 256.78024884 190.50000000 1.03686755 0.76923077 0.07162945 100.00000000 71629.45 c_{44} : 59.46475943 50.80000000 0.90043549 0.76923077 0.01721468 100.00000000 17214.68 c_{12} : 97.32695765 86.90000000 0.86152923 0.76923077 0.00851901 100.00000000 8519.01 c_{13} : 79.57600099 68.30000000 0.89622706 0.76923077 0.01612806 10.00000000 1612.81 M_{freq0}: 2.97174880 2.85858719 0.21658053 0.20833333 0.00006802 0.10000000 0.07 M_{freq1}: 2.97174881 2.85858719 0.21658053 0.20833333 0.00006802 0.10000000 0.07 M_{freq2}: 2.97174881 2.85858719 0.21658053 0.20833333 0.00006802

0.10000000 0.07 M_{freq3}: 2.97174882 2.85858719 0.21658053 0.20833333 0.00006802 0.10000000 0.07 M_{freq4}: 6.47507794 5.66706047 0.23803779 0.20833333 0.00088235 0.10000000 0.88 M_{freq5}: 6.47507794 5.66706047 0.23803779 0.20833333 0.00088235 0.10000000 0.88 H_{freq0}: 4.07088683 4.80643423 0.17645127 0.20833333 0.00101647 0.10000000 1.02 H_{freq1}: 4.07088683 5.58010025 0.15198677 0.20833333 0.00317494 0.10000000 3.17 H_{freq2}: 7.12197475 5.65316738 0.26246255 0.20833333 0.00292997 0.10000000 2.93 H_{freq3}: 7.12197475 6.36651842 0.23305434 0.20833333 0.00061113 0.10000000 0.61 H_{freq4}: 8.92842683 6.40050186 0.29061611 0.20833333 0.00677045 0.10000000 6.77 H_{freq5}: 8.92842683 7.64082373 0.24344089 0.20833333 0.00123254 0.10000000 1.23 bandw. G: 5.10621848 5.87085872 1.44959444 1.66666667 0.04712035 15.00000000 7068.05 bandw. K: 6.27902966 4.97424321 1.14755321 0.90909091 0.05686427 15.00000000 8529.64 bandw. M: 7.04639103 7.78109872 1.50929650 1.66666667 0.02476537 15.00000000 3714.81 bandw. L: 5.79466681 6.34433701 1.52226750 1.66666667 0.02085112 15.00000000 3127.67 bandw. H: 4.80961427 9.70902614 0.45034142 0.90909091 0.21045109 5.00000000 10522.55 $DOSerr_h$: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000 0.00 $DOSerr_o$: 98.86547597 0.00000000 98.86547597 0.00000000 9774.38233945 0.00000000 0.00 E_{prisf}: 109.76244599 220.00000000 109.76244599 220.00000000 12152.31831491 0.01000000 1215231.83

PARAMETERS b2=905445972.6509201527 m2=-15.9446815961 p2=0.0000000000 fdd=0.2648249504 qdds=0.5697753882 qddp=0.5648597117 qddd=0.8213593849 b0=47.7899139676 p0=1.1088003756 b1=-3.93 45715688 p1=0.6568823915 ndt=2.0000000000 cr1=-6.0000000000 cr2=3.2217589360 r1dd=6.5000000000 rcdd=10.0000000000 cr3=-1.1418272350 rmaxhm=10.1000000000 npar=18 VARGS -vb2=905445972.6509201527 -vm2=-15.9446815961 -vp2=0.0000000000 -vfdd=0.2648249504 -vqdds=0.5697753882 -vqddp=0.5648597117 -vqddd=0.8213593849 -vb0=47.7899139676 -vp0=1 .1088003756 -vb1=-3.9345715688 -vp1=0.6568823915 -vndt=2.0000000000 -vcr1=-6.0000000000 -vcr2=3.2217589360 -vr1dd=6.5000000000 -vrcdd=10.0000000000 -vcr3=-1.1418272350 -vrm axhm=10.1000000000

Quantity predicted target $norm_{pred}$ $norm_{tar}$ sq diff. weight objective * 100^2

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a_{hcp} : 5.57461126 5.57678969 5.57461126 5.57678969 0.00000475 1000.00000000 47.46 c/a : 1.58824164 1.58731122 15.42084557 15.41181168 0.00008161 100.00000000 81.61 a_{omega} : 8.91266648 8.73254342 1.11408331 1.09156793 0.00050694 10.00000000 50.69 c_{omega} : 5.40535546 5.32343103 0.67566943 0.66542888 0.00010487 10.00000000 10.49 a_{4h} : 5.56863112 5.56325146 1.00096700 1.00000000 0.00000094 1.00000000 0.01 c_{4h} : 18.04635261 17.75908031 1.01617608 1.00000000 0.00026167 1.00000000 2.62 a_{6h} : 5.56371838 5.54639384 1.00312357 1.00000000 0.00000976 1.00000000 0.10 c_{6h} : 27.13379120 26.77136353 1.01353789 1.00000000

0.00018327 1.00000000 1.83 a_{bcc} : 6.20079768 6.17948863 0.88582824 0.88278409 0.00000927 1.00000000 0.09 a_{fcc} : 7.85904307 7.88677000 1.12272044 1.12668143 0.00001569 1.00000000 0.16 DE(o,h) : 0.75090833 -0.63343333 0.05006056 -0.04222889 0.00851734 3000.00000000 255520.25 DE(4h,h): 2.02638500 3.17160000 0.00810554 0.01268640 0.00002098 2000.00000000 419.69 DE(6h,h): 3.02486000 3.72005000 0.01209944 0.01488020 0.00000773 2000.00000000 154.65 DE(b,h) : 7.76340500 7.63520000 0.07841823 0.07712323 0.00000168 1.00000000 0.02 DE(f,h) : 4.54128500 4.51880000 0.04587157 0.04564444 0.00000005 2000.00000000 1.03 c_{11} : 209.20671277 176.10000000 0.91384577 0.76923077 0.02091350 100.00000000 20913.50 c_{33} : 248.51083574 190.50000000 1.00347602 0.76923077 0.05487084 100.00000000 54870.84 c_{44} : 57.70646584 50.80000000 0.87381081 0.76923077 0.01093698 100.00000000 10936.98 c_{12} : 96.52645635 86.90000000 0.85444327 0.76923077 0.00726117 100.00000000 7261.17 c_{13} : 77.57509665 68.30000000 0.87369182 0.76923077 0.01091211 10.00000000 1091.21 M_{freq0}: 2.90595602 2.85858719 0.21178557 0.20833333 0.00001192 0.10000000 0.01 M_{freq1}: 2.90595603 2.85858719 0.21178557 0.20833333 0.00001192 0.10000000 0.01 M_{freq2}: 2.90595603 2.85858719 0.21178557 0.20833333 0.00001192 0.10000000 0.01 M_{freq3}: 2.90595604 2.85858719 0.21178557 0.20833333 0.00001192 0.10000000 0.01 M_{freq4}: 6.32257889 5.66706047 0.23243160 0.20833333 0.00058073 0.10000000 0.58 M_{freq5}: 6.32257889 5.66706047 0.23243160 0.20833333 0.00058073 0.10000000 0.58 H_{freq0}: 3.99946914 4.80643423 0.17335569 0.20833333 0.00122344 0.10000000 1.22 H_{freq1}: 3.99946914 5.58010025 0.14932039 0.20833333 0.00348253 0.10000000 3.48 H_{freq2}: 6.95348945 5.65316738 0.25625345 0.20833333 0.00229634 0.10000000 2.30 H_{freq3}: 6.95348945 6.36651842 0.22754095 0.20833333 0.00036893 0.10000000 0.37 H_{freq4}: 8.72200055 6.40050186 0.28389703 0.20833333 0.00570987 0.10000000 5.71 H_{freq5}: 8.72200055 7.64082373 0.23781251 0.20833333 0.00086902 0.10000000 0.87 bandw. G: 5.04499284 5.87085872 1.43221321 1.66666667 0.05496842 15.00000000 8245.26 bandw. K: 6.21100117 4.97424321 1.13512035 0.90909091 0.05108931 15.00000000 7663.40 bandw. M: 6.98652596 7.78109872 1.49647374 1.66666667 0.02896563 15.00000000 4344.84 bandw. L: 5.73616230 6.34433701 1.50689828 1.66666667 0.02552594 15.00000000 3828.89 bandw. H: 4.76063375 9.70902614 0.44575520 0.90909091 0.21467998 5.00000000 10734.00 $DOSerr_h$: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000 0.00 $DOSerr_o$: 106.23490802 0.00000000 106.23490802 0.00000000 11285.85568098 0.00000000 0.00 E_{prisf}: 94.24578590 220.00000000 94.24578590 220.00000000 15814.12236427 0.01000000 1581412.24

PARAMETERS b2=997988120.0035278797 m2=-15.4004196434 p2=0.0000000000 fdd=0.2648249504 qdds=0.5697753882 qddp=0.5648597117 qddd=0.8213593849 b0=53.3178751943 p0=1.1084242896 b1=-4.81 02743429 p1=0.6630121162 ndt=2.0000000000 cr1=-6.0000000000 cr2=3.2217589360 r1dd=6.5000000000

rcdd=10.0000000000 cr3=-1.1418272350 rmaxhm=10.1000000000 npar=18
VARGS -vb2=997988120.0035278797 -vm2=-15.4004196434 -vp2=0.0000000000 -vfdd=0.2648249504 -vqdds=0.5697753882 -vqddp=0.5648597117 -vqddd=0.8213593849 -vb0=53.3178751943 -vp0=1 .1084242896 -vb1=-4.8102743429 -vp1=0.6630121162 -vndt=2.0000000000 -vcr1=-6.0000000000 -vcr2=3.2217589360 -vr1dd=6.5000000000 -vrcdd=10.0000000000 -vcr3=-1.1418272350 -vrm axhm=10.1000000000

Quantity predicted target $\mathrm{norm}_{\mathrm{pred}}$ $\mathrm{norm}_{\mathrm{tar}}$ sq diff. weight objective * 100^2

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a_{hcp} : 5.63778583 5.57678969 5.63778583 5.57678969 0.00372053 1000.00000000 37205.29 c/a : 1.60080459 1.58731122 15.54282399 15.41181168 0.01716423 100.00000000 17164.23 a_{omega} : 9.04280677 8.73254342 1.13035085 1.09156793 0.00150411 10.00000000 150.41 c_{omega} : 5.44646765 5.32343103 0.68080846 0.66542888 0.00023653 10.00000000 23.65 a_{4h} : 5.63101774 5.56325146 1.01218106 1.00000000 0.00014838 1.00000000 1.48 c_{4h} : 18.26169876 17.75908031 1.02830205 1.00000000 0.00080101 1.00000000 8.01 a_{6h} : 5.62716702 5.54639384 1.01456319 1.00000000 0.00021209 1.00000000 2.12 c_{6h} : 27.45232488 26.77136353 1.02543618 1.00000000 0.00064700 1.00000000 6.47 a_{bcc} : 6.20079768 6.17948863 0.88582824 0.88278409 0.00000927 1.00000000 0.09 a_{fcc} : 7.94992578 7.88677000 1.13570368 1.12668143 0.00008140 1.00000000 0.81 DE(o,h) : 2.48206667 -0.63343333 0.16547111 -0.04222889 0.04313929 3000.00000000 1294178.70 DE(4h,h): 2.01600500 3.17160000 0.00806402 0.01268640 0.00002137 2000.00000000 427.33 DE(6h,h): 3.00347000 3.72005000 0.01201388 0.01488020 0.00000822 2000.00000000 164.32 DE(b,h) : 8.86714000 7.63520000 0.08956707 0.07712323 0.00015485 1.00000000 1.55 DE(f,h) : 4.51670000 4.51880000 0.04562323 0.04564444 0.00000000 2000.00000000 0.01 c_{11} : 247.46650824 176.10000000 1.08097020 0.76923077 0.09718147 100.00000000 97181.47 c_{33} : 292.48964963 190.50000000 1.18106057 0.76923077 0.16960378 100.00000000 169603.78 c_{44} : 67.56639226 50.80000000 1.02311315 0.76923077 0.06445626 100.00000000 64456.26 c_{12} : 126.49949516 86.90000000 1.11976184 0.76923077 0.12287203 100.00000000 122872.03 c_{13} : 86.58455848 68.30000000 0.97516115 0.76923077 0.04240732 10.00000000 4240.73 M_{freq0}: 3.27389129 2.85858719 0.23860062 0.20833333 0.00091611 0.10000000 0.92 M_{freq1}: 3.27389130 2.85858719 0.23860062 0.20833333 0.00091611 0.10000000 0.92 M_{freq2}: 3.27389130 2.85858719 0.23860062 0.20833333 0.00091611 0.10000000 0.92 M_{freq3}: 3.27389132 2.85858719 0.23860063 0.20833333 0.00091611 0.10000000 0.92 M_{freq4}: 7.17344228 5.66706047 0.26371117 0.20833333 0.00306670 0.10000000 3.07 M_{freq5}: 7.17344228 5.66706047 0.26371117 0.20833333 0.00306670 0.10000000 3.07 H_{freq0}: 4.80388952 4.80643423 0.20822303 0.20833333 0.00000001 0.10000000 0.00 H_{freq1}: 4.80388952 5.58010025 0.17935347 0.20833333 0.00083983 0.10000000 0.84 H_{freq2}: 7.98041792 5.65316738 0.29409833 0.20833333 0.00735563

0.10000000 7.36 H_{freq3}: 7.98041792 6.36651842 0.26114541 0.20833333 0.00278912 0.10000000 2.79 H_{freq4}: 9.75868685 6.40050186 0.31764068 0.20833333 0.01194810 0.10000000 11.95 H_{freq5}: 9.75868685 7.64082373 0.26607861 0.20833333 0.00333452 0.10000000 3.33 bandw. G: 4.80417199 5.87085872 1.36384704 1.66666667 0.09169972 15.00000000 13754.96 bandw. K: 5.93888721 4.97424321 1.08538890 0.90909091 0.03108098 15.00000000 4662.15 bandw. M: 6.74570510 7.78109872 1.44489130 1.66666667 0.04918431 15.00000000 7377.65 bandw. L: 5.47221176 6.34433701 1.43755808 1.66666667 0.05249074 15.00000000 7873.61 bandw. H: 4.57287512 9.70902614 0.42817468 0.90909091 0.23128042 5.00000000 11564.02 $DOSerr_h$: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000 0.00 $DOSerr_o$: 77.64288259 0.00000000 77.64288259 0.00000000 6028.41721726 0.00000000 0.00 E_{prisf}: 222.07696896 220.00000000 222.07696896 220.00000000 4.31380004 0.01000000 431.38

b2=0.0000000000 m2=0.0000000000 p2=0.0000000000 fdd=0.2648249504 qdds=0.5697753882 qddp=0.5648597117 qddd=0.8213593849 b0=59.5259478032 p0=1.1493643262 b1=-4.5351789513 p 1=0.6943513856 ndt=2.0000000000 cr1=-6.0000000000 cr2=3.2217589360 r1dd=6.5000000000 rcdd=10.0000000000 cr3=-1.1418272350 rmaxhm=10.1000000000 npar=18

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a_{hcp} : 5.62308140 5.57678969 5.62308140 5.57678969 0.00214292 1000.00000000 21429.23 c/a : 1.60706613 1.58731122 15.60361970 15.41181168 0.03679032 100.00000000 36790.32 a_{omega} : 8.95511122 8.73254342 1.11938890 1.09156793 0.00077401 10.00000000 77.40 c_{omega} : 5.44595238 5.32343103 0.68074405 0.66542888 0.00023455 10.00000000 23.46 a_{4h} : 5.61681826 5.56325146 1.00962869 1.00000000 0.00009271 1.00000000 0.93 c_{4h} : 18.20540238 17.75908031 1.02513205 1.00000000 0.00063162 1.00000000 6.32 a_{6h} : 5.61197437 5.54639384 1.01182399 1.00000000 0.00013981 1.00000000 1.40 c_{6h} : 27.37377796 26.77136353 1.02250219 1.00000000 0.00050635 1.00000000 5.06 a_{bcc} : 6.20079768 6.17948863 0.88582824 0.88278409 0.00000927 1.00000000 0.09 a_{fcc} : 7.92759020 7.88677000 1.13251289 1.12668143 0.00003401 1.00000000 0.34 DE(o,h) : -0.34139500 -0.63343333 -0.02275967 -0.04222889 0.00037905 3000.00000000 11371.52 DE(4h,h): 1.90152000 3.17160000 0.00760608 0.01268640 0.00002581 2000.00000000 516.19 DE(6h,h): 2.85588500 3.72005000 0.01142354 0.01488020 0.00001195 2000.00000000 238.97 DE(b,h) : 6.94059500 7.63520000 0.07010702 0.07712323 0.00004923 1.00000000 0.49 DE(f,h) : 4.30125500 4.51880000 0.04344702 0.04564444 0.00000483 2000.00000000 96.57 c_{11} : 184.83130888 176.10000000 0.80737041 0.76923077 0.00145463 100.00000000 1454.63 c_{33} : 210.64384444 190.50000000 0.85057074 0.76923077 0.00661619 100.00000000 6616.19 c_{44} : 49.26324195 50.80000000 0.74596066 0.76923077 0.00054150 100.00000000 541.50 c_{12} : 93.83944584 86.90000000 0.83065810 0.76923077 0.00377332 100.00000000 3773.32 c_{13}

: 67.50316906 68.30000000 0.76025644 0.76923077 0.00008054 10.00000000
8.05 M_{freq0}: 2.62482946 2.85858719 0.19129711 0.20833333 0.00029023 0.10000000
0.29 M_{freq1}: 2.62482947 2.85858719 0.19129711 0.20833333 0.00029023 0.10000000
0.29 M_{freq2}: 2.62482947 2.85858719 0.19129711 0.20833333 0.00029023 0.10000000
0.29 M_{freq3}: 2.62482948 2.85858719 0.19129711 0.20833333 0.00029023 0.10000000
0.29 M_{freq4}: 5.69996224 5.66706047 0.20954287 0.20833333 0.00000146 0.10000000
0.00 M_{freq5}: 5.69996224 5.66706047 0.20954287 0.20833333 0.00000146 0.10000000
0.00 H_{freq0}: 3.74539370 4.80643423 0.16234288 0.20833333 0.00211512 0.10000000
2.12 H_{freq1}: 3.74539370 5.58010025 0.13983447 0.20833333 0.00469209 0.10000000
4.69 H_{freq2}: 6.26248075 5.65316738 0.23078805 0.20833333 0.00050421 0.10000000
0.50 H_{freq3}: 6.26248075 6.36651842 0.20492888 0.20833333 0.00001159 0.10000000
0.01 H_{freq4}: 7.87194364 6.40050186 0.25622807 0.20833333 0.00229391 0.10000000
2.29 H_{freq5}: 7.87194364 7.64082373 0.21463501 0.20833333 0.00003971 0.10000000
0.04 bandw. G: 4.85859478 5.87085872 1.37929702 1.66666667 0.08258131 15.00000000 12387.20 bandw. K: 6.00147342 4.97424321 1.09682713 0.90909091 0.03524489 15.00000000 5286.73 bandw. M: 6.80148846 7.78109872 1.45683977 1.66666667 0.04402732 15.00000000 6604.10 bandw. L: 5.52527398 6.34433701 1.45149760 1.66666667 0.04629772 15.00000000 6944.66 bandw. H: 4.61641335 9.70902614 0.43225132 0.90909091 0.22737599 5.00000000 11368.80 $DOSerr_h$: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000 0.00 $DOSerr_o$: 110.29822598 0.00000000 110.29822598 0.00000000 12165.69865409 0.00000000 0.00 E_{prisf}: 70.80322562 220.00000000 70.80322562 220.00000000 22259.67748515 0.00100000 222596.77

b2=529957467.2048873901 m2=-15.8531159425 p2=0.0000000000 fdd=0.2648249504 qdds=0.5697753882 qddp=0.5648597117 qddd=0.8213593849 b0=47.1964963231 p0=1.0523246525 b1=-4.93 66489527 p1=0.6329489051 ndt=2.0000000000 cr1=-6.0000000000 cr2=3.2217589360 r1dd=6.5000000000 rcdd=10.0000000000 cr3=-1.1418272350 rmaxhm=10.1000000000 npar=18

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a_{hcp} : 5.57188821 5.57678969 5.57188821 5.57678969 0.00002402 1000.00000000 240.24 c/a : 1.58940570 1.58731122 15.43214786 15.41181168 0.00041356 100.00000000 413.56 a_{omega} : 8.90037874 8.73254342 1.11254734 1.09156793 0.00044014 10.00000000 44.01 c_{omega} : 5.40408192 5.32343103 0.67551024 0.66542888 0.00010163 10.00000000 10.16 a_{4h} : 5.57268326 5.56325146 1.00169538 1.00000000 0.00000287 1.00000000 0.03 c_{4h} : 18.01242981 17.75908031 1.01426591 1.00000000 0.00020352 1.00000000 2.04 a_{6h} : 5.56660954 5.54639384 1.00364484 1.00000000 0.00001328 1.00000000 0.13 c_{6h} : 27.10263712 26.77136353 1.01237418 1.00000000 0.00015312 1.00000000 1.53 a_{bcc} : 6.20079768 6.17948863 0.88582824 0.88278409 0.00000927 1.00000000 0.09 a_{fcc} : 7.86058346 7.88677000 1.12294049 1.12668143 0.00001399 1.00000000 0.14 DE(o,h) : -0.49262667 -0.63343333 -

0.03284178 -0.04222889 0.00008812 3000.00000000 2643.54 DE(4h,h): 2.28232000 3.17160000 0.00912928 0.01268640 0.00001265 2000.00000000 253.06 DE(6h,h): 3.36564500 3.72005000 0.01346258 0.01488020 0.00000201 2000.00000000 40.19 DE(b,h) : 7.56147000 7.63520000 0.07637848 0.07712323 0.00000055 1.00000000 0.01 DE(f,h) : 5.02996000 4.51880000 0.05080768 0.04564444 0.00002666 2000.00000000 533.18 c_{11} : 199.75935696 176.10000000 0.87257833 0.76923077 0.01068072 100.00000000 10680.72 c_{33} : 257.57041942 190.50000000 1.04005822 0.76923077 0.07334751 100.00000000 73347.51 c_{44} : 57.74878709 50.80000000 0.87445165 0.76923077 0.01107143 100.00000000 11071.43 c_{12} : 99.00485786 86.90000000 0.87638185 0.76923077 0.01148135 100.00000000 11481.35 c_{13} : 78.58125619 68.30000000 0.88502372 0.76923077 0.01340801 10.00000000 1340.80 M_{freq0}: 2.89853526 2.85858719 0.21124474 0.20833333 0.00000848 0.10000000 0.01 M_{freq1}: 2.89853527 2.85858719 0.21124474 0.20833333 0.00000848 0.10000000 0.01 M_{freq2}: 2.89853527 2.85858719 0.21124474 0.20833333 0.00000848 0.10000000 0.01 M_{freq3}: 2.89853528 2.85858719 0.21124474 0.20833333 0.00000848 0.10000000 0.01 M_{freq4}: 6.67131393 5.66706047 0.24525185 0.20833333 0.00136298 0.10000000 1.36 M_{freq5}: 6.67131393 5.66706047 0.24525185 0.20833333 0.00136298 0.10000000 1.36 H_{freq0}: 3.83835538 4.80643423 0.16637227 0.20833333 0.00176073 0.10000000 1.76 H_{freq1}: 3.83835538 5.58010025 0.14330520 0.20833333 0.00422866 0.10000000 4.23 H_{freq2}: 7.48779156 5.65316738 0.27594382 0.20833333 0.00457118 0.10000000 4.57 H_{freq3}: 7.48779156 6.36651842 0.24502506 0.20833333 0.00134628 0.10000000 1.35 H_{freq4}: 9.36361994 6.40050186 0.30478144 0.20833333 0.00930224 0.10000000 9.30 H_{freq5}: 9.36361994 7.64082373 0.25530679 0.20833333 0.00220651 0.10000000 2.21 bandw. G: 5.05587740 5.87085872 1.43530320 1.66666667 0.05352905 15.00000000 8029.36 bandw. K: 6.22324630 4.97424321 1.13735827 0.90909091 0.05210599 15.00000000 7815.90 bandw. M: 6.99741052 7.78109872 1.49880515 1.66666667 0.02817749 15.00000000 4226.62 bandw. L: 5.74704686 6.34433701 1.50975767 1.66666667 0.02462043 15.00000000 3693.07 bandw. H: 4.77015774 9.70902614 0.44664696 0.90909091 0.21385440 5.00000000 10692.72 $DOSerr_h$: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000 0.00 $DOSerr_o$: 104.85200112 0.00000000 104.85200112 0.00000000 10993.94213887 0.00000000 0.00 E_{prisf}: 72.80642405 220.00000000 72.80642405 220.00000000 21665.94880152 0.00100000 216659.49

b2=238992966.9478154778 m2=-15.0156845030 p2=0.0000000000 fdd=0.2648249504 qdds=0.5697753882 qddp=0.5648597117 qddd=0.8213593849 b0=47.0500980357 p0=1.0556839408 b1=-5.13 00359501 p1=0.6507410387 ndt=2.0000000000 cr1=-6.0000000000 cr2=3.2217589360 r1dd=6.5000000000 rcdd=10.0000000000 cr3=-1.1418272350 rmaxhm=10.1000000000 npar=18

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a_{hcp} : 5.65153719 5.57678969 5.65153719 5.57678969 0.00558719 1000.00000000

55871.89 c/a : 1.59497837 1.58731122 15.48625502 15.41181168 0.00554181 100.00000000 5541.81 a_{omega} : 9.03327448 8.73254342 1.12915931 1.09156793 0.00141311 10.00000000 141.31 c_{omega} : 5.46261177 5.32343103 0.68282647 0.66542888 0.00030268 10.00000000 30.27 a_{4h} : 5.65046462 5.56325146 1.01567665 1.00000000 0.00024576 1.00000000 2.46 c_{4h} : 18.28532568 17.75908031 1.02963247 1.00000000 0.00087808 1.00000000 8.78 a_{6h} : 5.64546730 5.54639384 1.01786268 1.00000000 0.00031908 1.00000000 3.19 c_{6h} : 27.50655214 26.77136353 1.02746175 1.00000000 0.00075415 1.00000000 7.54 a_{bcc} : 6.20079768 6.17948863 0.88582824 0.88278409 0.00000927 1.00000000 0.09 a_{fcc} : 7.97380174 7.88677000 1.13911453 1.12668143 0.00015458 1.00000000 1.55 DE(o,h) : -0.27297000 -0.63343333 -0.01819800 -0.04222889 0.00057748 3000.00000000 17324.51 DE(4h,h): 2.06699250 3.17160000 0.00826797 0.01268640 0.00001952 2000.00000000 390.45 DE(6h,h): 3.06958667 3.72005000 0.01227835 0.01488020 0.00000677 2000.00000000 135.39 DE(b,h) : 7.84221000 7.63520000 0.07921424 0.07712323 0.00000437 1.00000000 0.04 DE(f,h) : 4.60577000 4.51880000 0.04652293 0.04564444 0.00000077 2000.00000000 15.43 c_{11} : 200.13394216 176.10000000 0.87421457 0.76923077 0.01102160 100.00000000 11021.60 c_{33} : 238.53684776 190.50000000 0.96320148 0.76923077 0.03762464 100.00000000 37624.64 c_{44} : 54.80421660 50.80000000 0.82986397 0.76923077 0.00367639 100.00000000 3676.39 c_{12} : 111.18853892 86.90000000 0.98423067 0.76923077 0.04622496 100.00000000 46224.96 c_{13} : 72.65583597 68.30000000 0.81828850 0.76923077 0.00240666 10.00000000 240.67 M_{freq0}: 2.84168323 2.85858719 0.20710138 0.20833333 0.00000152 0.10000000 0.00 M_{freq1}: 2.84168324 2.85858719 0.20710138 0.20833333 0.00000152 0.10000000 0.00 M_{freq2}: 2.84168324 2.85858719 0.20710138 0.20833333 0.00000152 0.10000000 0.00 M_{freq3}: 2.84168325 2.85858719 0.20710138 0.20833333 0.00000152 0.10000000 0.00 M_{freq4}: 6.35692654 5.66706047 0.23369429 0.20833333 0.00064318 0.10000000 0.64 M_{freq5}: 6.35692654 5.66706047 0.23369429 0.20833333 0.00064318 0.10000000 0.64 H_{freq0}: 4.05308243 4.80643423 0.17567954 0.20833333 0.00106627 0.10000000 1.07 H_{freq1}: 4.05308243 5.58010025 0.15132204 0.20833333 0.00325029 0.10000000 3.25 H_{freq2}: 7.14466972 5.65316738 0.26329892 0.20833333 0.00302122 0.10000000 3.02 H_{freq3}: 7.14466972 6.36651842 0.23379699 0.20833333 0.00064840 0.10000000 0.65 H_{freq4}: 8.81982929 6.40050186 0.28708131 0.20833333 0.00620124 0.10000000 6.20 H_{freq5}: 8.81982929 7.64082373 0.24047989 0.20833333 0.00103340 0.10000000 1.03 bandw. G: 4.75383090 5.87085872 1.34955581 1.66666667 0.10055929 15.00000000 15083.89 bandw. K: 5.88038270 4.97424321 1.07469664 0.90909091 0.02742526 15.00000000 4113.79 bandw. M: 6.69400345 7.78109872 1.43381710 1.66666667 0.05421892 15.00000000 8132.84 bandw. L: 5.42187068 6.34433701 1.42433340 1.66666667 0.05872541 15.00000000 8808.81 bandw. H: 4.53341860 9.70902614 0.42448023 0.90909091 0.23484751 5.00000000 11742.38 $DOSerr_h$: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000

0.00 $DOSerr_o$: 106.26772307 0.00000000 106.26772307 0.00000000 11292.82896546 0.00000000 0.00 E_{prisf}: 105.96058776 220.00000000 105.96058776 220.00000000 13004.98754412 0.00100000 130049.88

b2=0.0000000000 m2=0.0000000000 p2=0.0000000000 fdd=0.2648249504 qdds=0.5697753882 qddp=0.5648597117 qddd=0.8213593849 b0=140.6250881140 p0=1.5000000000 b1=-0.3349120798 p1=0.5103314042 ndt=2.0000000000 cr1=-6.0000000000 cr2=3.2217589360 r1dd=6.5000000000 rcdd=10.0000000000 cr3=-1.1418272350 rmaxhm=10.1000000000 npar=18

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a_{hcp} : 5.56058759 5.57678969 5.56058759 5.57678969 0.00026251 1000.00000000 2625.08 c/a : 1.59424873 1.58731122 15.47917067 15.41181168 0.00453723 100.00000000 4537.23 a_{omega} : 8.85711014 8.73254342 1.10713877 1.09156793 0.00024245 10.00000000 24.25 c_{omega} : 5.41409627 5.32343103 0.67676203 0.66542888 0.00012844 10.00000000 12.84 a_{4h} : 5.54693871 5.56325146 0.99706777 1.00000000 0.00000860 1.00000000 0.09 c_{4h} : 18.02419033 17.75908031 1.01492814 1.00000000 0.00022285 1.00000000 2.23 a_{6h} : 5.54272137 5.54639384 0.99933786 1.00000000 0.00000044 1.00000000 0.00 c_{6h} : 27.08087241 26.77136353 1.01156119 1.00000000 0.00013366 1.00000000 1.34 a_{bcc} : 6.20079768 6.17948863 0.88582824 0.88278409 0.00000927 1.00000000 0.09 a_{fcc} : 7.83131615 7.88677000 1.11875945 1.12668143 0.00006276 1.00000000 0.63 DE(o,h) : 1.24301500 -0.63343333 0.08286767 -0.04222889 0.01564915 3000.00000000 469474.45 DE(4h,h): 1.72554000 3.17160000 0.00690216 0.01268640 0.00003346 2000.00000000 669.15 DE(6h,h): 2.63205667 3.72005000 0.01052823 0.01488020 0.00001894 2000.00000000 378.79 DE(b,h) : 8.05059500 7.63520000 0.08131914 0.07712323 0.00001761 1.00000000 0.18 DE(f,h) : 3.97823500 4.51880000 0.04018419 0.04564444 0.00002981 2000.00000000 596.29 c_{11} : 192.43892517 176.10000000 0.84060160 0.76923077 0.00509380 100.00000000 5093.80 c_{33} : 204.85827777 190.50000000 0.82720887 0.76923077 0.00336146 100.00000000 3361.46 c_{44} : 50.34135405 50.80000000 0.76228580 0.76923077 0.00004823 100.00000000 48.23 c_{12} : 75.61328960 86.90000000 0.66932185 0.76923077 0.00998179 100.00000000 9981.79 c_{13} : 68.71389026 68.30000000 0.77389222 0.76923077 0.00002173 10.00000000 2.17 M_{freq0}: 2.67628898 2.85858719 0.19504747 0.20833333 0.00017651 0.10000000 0.18 M_{freq1}: 2.67628899 2.85858719 0.19504747 0.20833333 0.00017651 0.10000000 0.18 M_{freq2}: 2.67628899 2.85858719 0.19504747 0.20833333 0.00017651 0.10000000 0.18 M_{freq3}: 2.67628900 2.85858719 0.19504747 0.20833333 0.00017651 0.10000000 0.18 M_{freq4}: 5.25767874 5.66706047 0.19328358 0.20833333 0.00022650 0.10000000 0.23 M_{freq5}: 5.25767874 5.66706047 0.19328358 0.20833333 0.00022650 0.10000000 0.23 H_{freq0}: 3.63161265 4.80643423 0.15741107 0.20833333 0.00259308 0.10000000 2.59 H_{freq1}: 3.63161265 5.58010025 0.13558645 0.20833333 0.00529211 0.10000000 5.29 H_{freq2}: 5.48887273 5.65316738 0.20227867 0.20833333 0.00003666 0.10000000

0.04 H_{freq3}: 5.48887273 6.36651842 0.17961389 0.20833333 0.00082481 0.10000000 0.82 H_{freq4}: 7.13585316 6.40050186 0.23226867 0.20833333 0.00057290 0.10000000 0.57 H_{freq5}: 7.13585316 7.64082373 0.19456490 0.20833333 0.00018957 0.10000000 0.19 bandw. G: 5.10077620 5.87085872 1.44804944 1.66666667 0.04779349 15.00000000 7169.02 bandw. K: 6.27358738 4.97424321 1.14655858 0.90909091 0.05639090 15.00000000 8458.63 bandw. M: 7.04094875 7.78109872 1.50813079 1.66666667 0.02513362 15.00000000 3770.04 bandw. L: 5.78922453 6.34433701 1.52083780 1.66666667 0.02126606 15.00000000 3189.91 bandw. H: 4.80417199 9.70902614 0.44983184 0.90909091 0.21091889 5.00000000 10545.94 $DOSerr_h$: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000 0.00 $DOSerr_o$: 101.31732878 0.00000000 101.31732878 0.00000000 10265.20111043 0.00000000 0.00 E_{prisf}: 51.15374553 220.00000000 51.15374553 220.00000000 28509.05764790 0.00100000 285090.58

b2=0.0000000000 m2=0.0000000000 p2=0.0000000000 fdd=0.2648249504 qdds=0.5697753882 qddp=0.5648597117 qddd=0.8213593849 b0=114.1564941581 p0=1.3883912590 b1=-1.8695661213 p1=0.7021069541 ndt=2.0000000000 cr1=-6.0000000000 cr2=3.2217589360 r1dd=6.5000000000 rcdd=10.0000000000 cr3=-1.1418272350 rmaxhm=10.1000000000 npar=18

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a_{hcp} : 5.62641713 5.57678969 5.62641713 5.57678969 0.00246288 1000.00000000 24628.83 c/a : 1.60564282 1.58731122 15.58980022 15.41181168 0.03167992 100.00000000 31679.92 a_{omega} : 8.96538123 8.73254342 1.12067265 1.09156793 0.00084709 10.00000000 84.71 c_{omega} : 5.45575817 5.32343103 0.68196977 0.66542888 0.00027360 10.00000000 27.36 a_{4h} : 5.61278398 5.56325146 1.00890352 1.00000000 0.00007927 1.00000000 0.79 c_{4h} : 18.24121329 17.75908031 1.02714853 1.00000000 0.00073704 1.00000000 7.37 a_{6h} : 5.60912152 5.54639384 1.01130963 1.00000000 0.00012791 1.00000000 1.28 c_{6h} : 27.40562165 26.77136353 1.02369166 1.00000000 0.00056129 1.00000000 5.61 a_{bcc} : 6.20079768 6.17948863 0.88582824 0.88278409 0.00000927 1.00000000 0.09 a_{fcc} : 7.92527962 7.88677000 1.13218280 1.12668143 0.00003027 1.00000000 0.30 DE(o,h) : 1.26412500 -0.63343333 0.08427500 -0.04222889 0.01600323 3000.00000000 480097.02 DE(4h,h): 1.69892000 3.17160000 0.00679568 0.01268640 0.00003470 2000.00000000 694.01 DE(6h,h): 2.59242333 3.72005000 0.01036969 0.01488020 0.00002034 2000.00000000 406.89 DE(b,h) : 7.56535500 7.63520000 0.07641773 0.07712323 0.00000050 1.00000000 0.00 DE(f,h) : 3.93098500 4.51880000 0.03970692 0.04564444 0.00003525 2000.00000000 705.08 c_{11} : 195.05516670 176.10000000 0.85202973 0.76923077 0.00685567 100.00000000 6855.67 c_{33} : 206.27436836 190.50000000 0.83292699 0.76923077 0.00405721 100.00000000 4057.21 c_{44} : 49.63461769 50.80000000 0.75158416 0.76923077 0.00031140 100.00000000 311.40 c_{12} : 86.92490619 86.90000000 0.76945124 0.76923077 0.00000005 100.00000000 0.05 c_{13} : 68.73179082

68.30000000 0.77409383 0.76923077 0.00002365 10.00000000 2.36 M_{freq0}: 2.68061683 2.85858719 0.19536288 0.20833333 0.00016823 0.10000000 0.17 M_{freq1}: 2.68061684 2.85858719 0.19536289 0.20833333 0.00016823 0.10000000 0.17 M_{freq2}: 2.68061684 2.85858719 0.19536289 0.20833333 0.00016823 0.10000000 0.17 M_{freq3}: 2.68061685 2.85858719 0.19536289 0.20833333 0.00016823 0.10000000 0.17 M_{freq4}: 5.45403129 5.66706047 0.20050192 0.20833333 0.00006133 0.10000000 0.06 M_{freq5}: 5.45403129 5.66706047 0.20050192 0.20833333 0.00006133 0.10000000 0.06 H_{freq0}: 3.89335853 4.80643423 0.16875636 0.20833333 0.00156634 0.10000000 1.57 H_{freq1}: 3.89335853 5.58010025 0.14535874 0.20833333 0.00396580 0.10000000 3.97 H_{freq2}: 5.77373518 5.65316738 0.21277656 0.20833333 0.00001974 0.10000000 0.02 H_{freq3}: 5.77373518 6.36651842 0.18893552 0.20833333 0.00037627 0.10000000 0.38 H_{freq4}: 7.33883803 6.40050186 0.23887574 0.20833333 0.00093284 0.10000000 0.93 H_{freq5}: 7.33883803 7.64082373 0.20009945 0.20833333 0.00006780 0.10000000 0.07 bandw. G: 4.84634965 5.87085872 1.37582078 1.66666667 0.08459133 15.00000000 12688.70 bandw. K: 5.98650715 4.97424321 1.09409190 0.90909091 0.03422537 15.00000000 5133.81 bandw. M: 6.78924333 7.78109872 1.45421694 1.66666667 0.04513489 15.00000000 6770.23 bandw. L: 5.51302886 6.34433701 1.44828079 1.66666667 0.04769239 15.00000000 7153.86 bandw. H: 4.60552880 9.70902614 0.43123216 0.90909091 0.22834898 5.00000000 11417.45 $DOSerr_h$: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000 0.00 $DOSerr_o$: 106.36466941 0.00000000 106.36466941 0.00000000 11313.44289798 0.00000000 0.00 E_{prisf}: 92.22065278 220.00000000 92.22065278 220.00000000 16327.56157472 0.00100000 163275.62

b2=100000000.0000000000 m2=-17.0000000000 p2=0.0000000000 fdd=0.2648249504 qdds=0.5697753882 qddp=0.5648597117 qddd=0.8213593849 b0=69.7247791494 p0=1.1823996774 b1=-6.1008440394 p1=0.7500000000 ndt=2.0000000000 cr1=-6.0000000000 cr2=3.2217589360 r1dd=6.5000000000 rcdd=10.0000000000 cr3=-1.1418272350 rmaxhm=10.1000000000 npar=18

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a_{hcp} : 5.56276602 5.57678969 5.56276602 5.57678969 0.00019666 1000.00000000 1966.63 c/a : 1.59331360 1.58731122 15.47009117 15.41181168 0.00339650 100.00000000 3396.50 a_{omega} : 8.86570413 8.73254342 1.10821302 1.09156793 0.00027706 10.00000000 27.71 c_{omega} : 5.39008159 5.32343103 0.67376020 0.66542888 0.00006941 10.00000000 6.94 a_{4h} : 5.55263546 5.56325146 0.99809176 1.00000000 0.00000364 1.00000000 0.04 c_{4h} : 18.02391102 17.75908031 1.01491241 1.00000000 0.00022238 1.00000000 2.22 a_{6h} : 5.54842769 5.54639384 1.00036670 1.00000000 0.00000013 1.00000000 0.00 c_{6h} : 27.08910587 26.77136353 1.01186874 1.00000000 0.00014087 1.00000000 1.41 a_{bcc} : 6.20079768 6.17948863 0.88582824 0.88278409 0.00000927 1.00000000 0.09 a_{fcc} : 7.83901807 7.88677000 1.11985972 1.12668143 0.00004654 1.00000000 0.47 DE(o,h) : 0.70288333 -0.63343333

0.04685889 -0.04222889 0.00793663 3000.00000000 238098.96 DE(4h,h): 1.86685500 3.17160000 0.00746742 0.01268640 0.00002724 2000.00000000 544.76 DE(6h,h): 2.81596667 3.72005000 0.01126387 0.01488020 0.00001308 2000.00000000 261.56 DE(b,h) : 7.38194000 7.63520000 0.07456505 0.07712323 0.00000654 1.00000000 0.07 DE(f,h) : 4.24119000 4.51880000 0.04284030 0.04564444 0.00000786 2000.00000000 157.26 c_{11} : 208.93562758 176.10000000 0.91266163 0.76923077 0.02057241 100.00000000 20572.41 c_{33} : 237.98543138 190.50000000 0.96097489 0.76923077 0.03676581 100.00000000 36765.81 c_{44} : 54.28185458 50.80000000 0.82195419 0.76923077 0.00277976 100.00000000 2779.76 c_{12} : 97.64679227 86.90000000 0.86436038 0.76923077 0.00904964 100.00000000 9049.64 c_{13} : 74.24437438 68.30000000 0.83617946 0.76923077 0.00448213 10.00000000 448.21 M_{freq0}: 2.82856685 2.85858719 0.20614546 0.20833333 0.00000479 0.10000000 0.00 M_{freq1}: 2.82856686 2.85858719 0.20614546 0.20833333 0.00000479 0.10000000 0.00 M_{freq2}: 2.82856686 2.85858719 0.20614546 0.20833333 0.00000479 0.10000000 0.00 M_{freq3}: 2.82856687 2.85858719 0.20614546 0.20833333 0.00000479 0.10000000 0.00 M_{freq4}: 6.02957369 5.66706047 0.22166010 0.20833333 0.00017760 0.10000000 0.18 M_{freq5}: 6.02957369 5.66706047 0.22166010 0.20833333 0.00017760 0.10000000 0.18 H_{freq0}: 4.01647120 4.80643423 0.17409264 0.20833333 0.00117242 0.10000000 1.17 H_{freq1}: 4.01647120 5.58010025 0.14995516 0.20833333 0.00340801 0.10000000 3.41 H_{freq2}: 6.59737209 5.65316738 0.24312963 0.20833333 0.00121078 0.10000000 1.21 H_{freq3}: 6.59737209 6.36651842 0.21588762 0.20833333 0.00005707 0.10000000 0.06 H_{freq4}: 8.27795011 6.40050186 0.26944339 0.20833333 0.00373444 0.10000000 3.73 H_{freq5}: 8.27795011 7.64082373 0.22570511 0.20833333 0.00030178 0.10000000 0.30 bandw. G: 5.09125222 5.87085872 1.44534569 1.66666667 0.04898297 15.00000000 7347.45 bandw. K: 6.26406339 4.97424321 1.14481798 0.90909091 0.05556725 15.00000000 8335.09 bandw. M: 7.03142476 7.78109872 1.50609081 1.66666667 0.02578461 15.00000000 3867.69 bandw. L: 5.78242168 6.34433701 1.51905068 1.66666667 0.02179048 15.00000000 3268.57 bandw. H: 4.79736914 9.70902614 0.44919486 0.90909091 0.21150437 5.00000000 10575.22 $DOSerr_h$: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000 0.00 $DOSerr_o$: 105.23589358 0.00000000 105.23589358 0.00000000 11074.59329851 0.00000000 0.00 E_{prisf}: 94.86005764 220.00000000 94.86005764 220.00000000 15660.00517479 0.00100000 156600.05

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1.48627382 1.66666667 0.03254158 15.00000000 4881.24 bandw. L: 5.68990293 6.34433701 1.49474587 1.66666667 0.02955676 15.00000000 4433.51 bandw. H: 4.72389837 9.70902614 0.44231553 0.90909091 0.21787925 5.00000000 10893.96 $\mathrm{DOSerr_h}$: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000 0.00 $\mathrm{DOSerr_o}$: 103.15991133 0.00000000 103.15991133 0.00000000 10641.96730619 0.00000000 0.00 $\mathrm{E_{prisf}}$: 95.95221364 220.00000000 95.95221364 220.00000000 15387.85330116 1.00000000 153878533.01

1.4 TODO Gamma Surfaces for New Model

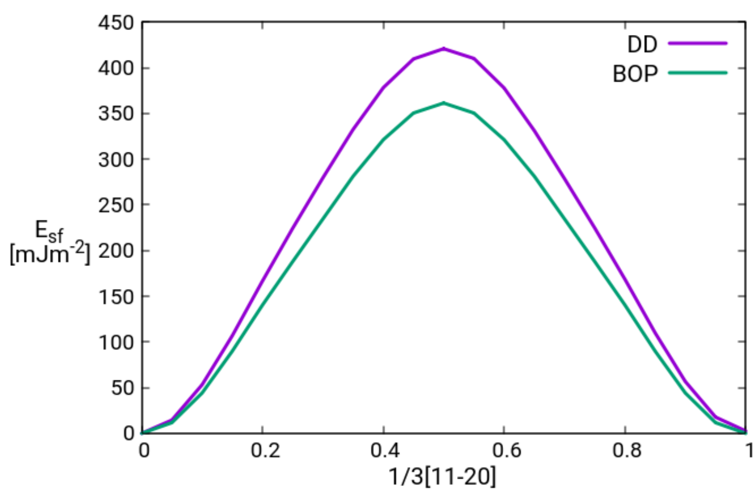
1.4.1 BOP

This was determined using non-periodicity along the z direction.

Initally the number of layers was not enough. This meant that the atoms which were at the interface of the stacking fault actually obtained the information of it's local atomic environment from some the atoms at the free surface, hence why the stacking fault energy was high as the energy from the free surfaces was contributing.

The number of layers was increased to 64 for both the basal and the prismatic stacking fault.

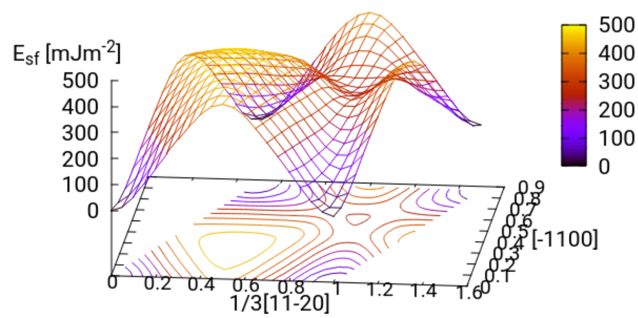
1. Basal gamma line

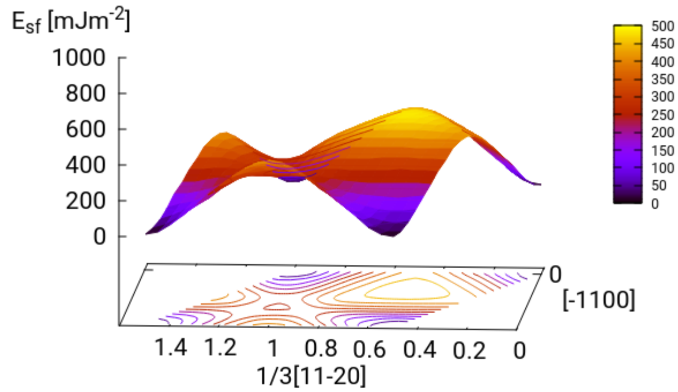


We can see that the gamma line from the bop model is consistently lower than that of the one from the direct-diagonalisation plot. This may be due to the fact that the number of layers in the BOP simulation was much higher (64 compared to 30), so that the actual interaction between the tight-binding fault surfaces under homogeneous shear boundary conditions had more of an effect on the stacking fault energy than the free surfaces in the BOP simulation.

2. Basal Gamma Surfaces

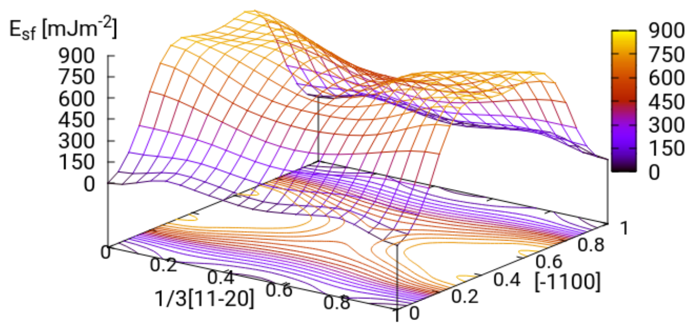
   (a) tbe

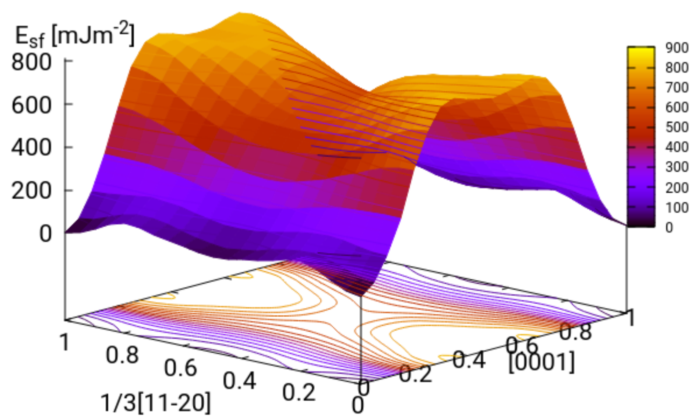




3. Prismatic Gamma Surfaces

(a) tbe





1.5 Final Model

fdd=0.2648249504 qdds=0.5697753882 qddp=0.5648597117 qddd=0.8213593849 b0=49.75575654 p0=1.105068573 b1=-5.09734161 p1=0.6991977165 cr2=3.221758936 cr3=-1.141827235 cr1=-6.0 ndt=2.0 r1dd=6.3741123381 rcdd=9.8768388324 rmaxhm=9.9756072207 VARGS -vfdd=0.2648249504 -vqdds=0.5697753882 -vqddp=0.5648597117 -vqddd=0.8213593849 -vb0=49.75575654 -vp0=1.105068573 -vb1=-5.09734161 -vp1=0.6991977165 -vcr2=3.221758936 -vcr3=-1.141827235 -vcr1=-6.0 -vndt=2.0 -vr1dd=6.3741123381 -vrcdd=9.8768388324 -vrmaxhm=9.9756072207

a_{hcp} : 5.55908396 5.57678969 5.55908396 5.57678969 0.00031349 1500.00000000 4702.39 c/a : 1.61268131 1.58731122 15.65813964 15.41181168 0.06067746 100.00000000 60677.46 a_{omega} : 8.84739387 8.73254342 1.10592423 1.09156793 0.00020610 10.00000000 20.61 c_{omega} : 5.38456249 5.32343103 0.67307031 0.66542888 0.00005839 10.00000000 5.84 a_{4h} : 5.55471471 5.56325146 0.99846551 1.00000000 0.00000235 1.00000000 0.02 c_{4h} : 17.98986999 17.75908031 1.01299559 1.00000000 0.00016889 1.00000000 1.69 a_{6h} : 5.54952123 5.54639384 1.00056386 1.00000000 0.00000032 1.00000000 0.00 c_{6h} : 27.05646584 26.77136353 1.01064953 1.00000000 0.00011341 1.00000000 1.13 a_{bcc} : 6.27665250 6.17948863 0.89666464 0.88278409 0.00019267 1.00000000 1.93 a_{fcc} : 7.83824788 7.88677000 1.11974970 1.12668143 0.00004805 1.00000000 0.48 DE(o,h) : -1.09765167 -0.63343333 -0.07317678 -0.04222889 0.00095777 3000.00000000 28733.15 DE(4h,h): 1.97809750 3.17160000 0.00791239 0.01268640 0.00002279 2000.00000000 455.82 DE(6h,h): 2.97676333 3.72005000 0.01190705 0.01488020 0.00000884 2000.00000000 176.79 DE(b,h) : 9.82662500 7.63520000 0.09925884 0.07712323 0.00048999 200.00000000 979.97 DE(f,h) : 4.48794500 4.51880000 0.04533278 0.04564444 0.00000010 2000.00000000 1.94 c_{11} : 180.67966452 176.10000000 0.78923542 0.76923077 0.00040019 100.00000000 400.19 c_{33} : 206.14770273 190.50000000 0.83241552 0.76923077 0.00399231 100.00000000 3992.31 c_{44} : 48.30576681 50.80000000 0.73146225 0.76923077 0.00142646 100.00000000 1426.46 c_{12} : 95.22633084 86.90000000 0.84293468 0.76923077 0.00543227 100.00000000 5432.27 c_{13} : 66.46772326 68.30000000 0.74859470 0.76923077 0.00042585 50.00000000 212.92 M_{freq0}: 2.52855122 2.85858719 0.18428037 0.20833333 0.00057855 0.10000000 0.58 M_{freq1}: 2.52855123 2.85858719 0.18428037 0.20833333 0.00057855 0.10000000 0.58 M_{freq2}: 2.52855123 2.85858719 0.18428037 0.20833333 0.00057855 0.10000000 0.58 M_{freq3}: 2.52855124 2.85858719 0.18428037 0.20833333 0.00057854 0.10000000 0.58 M_{freq4}: 5.59220819 5.66706047 0.20558160 0.20833333 0.00000757 0.10000000 0.01 M_{freq5}: 5.59220819 5.66706047 0.20558160 0.20833333 0.00000757 0.10000000 0.01 H_{freq0}: 3.57525560 4.80643423 0.15496829 0.20833333 0.00284783 0.10000000 2.85 H_{freq1}: 3.57525560 5.58010025 0.13348235 0.20833333 0.00560267 0.10000000 5.60 H_{freq2}: 6.11165910 5.65316738 0.22522990 0.20833333 0.00028549 0.10000000 0.29 H_{freq3}: 6.11165910 6.36651842 0.19999350 0.20833333 0.00006955 0.10000000 0.07 H_{freq4}: 7.75488320 6.40050186 0.25241781 0.20833333 0.00194344 0.10000000 1.94 H_{freq5}: 7.75488320 7.64082373 0.21144326 0.20833333 0.00000967 0.10000000 0.01 bandw. G: 5.03138714 5.87085872 1.42835071 1.66666667 0.05679449 1.00000000 567.94 bandw. K: 6.21236174 4.97424321 1.13536901

0.90909091 0.05120178 1.00000000 512.02 bandw. M: 7.05319388 7.78109872 1.51075363 1.66666667 0.02430888 1.00000000 243.09 bandw. L: 5.72119604 6.34433701 1.50296662 1.66666667 0.02679771 1.00000000 267.98 bandw. H: 4.78240287 9.70902614 0.44779352 0.90909091 0.21279528 1.00000000 2127.95 $\mathrm{DOSerr_h}$: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.10000000 0.00 $\mathrm{DOSerr_o}$: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.10000000 0.00

1.6 TODO Write first section of Literature review

1.6.1 TODO Summarise Stacking Faults and write review

1.6.2 TODO Write up the tight binding fitting of oxygen and an explanation for paramagnetism.

1.6.3 TODO Summarise dislocations and Oxygen interactions (review)

1.7 TODO See how the PDOS changes with addition of oxygen and how the tetrahedral/octahedral sites change this.

1.8 TODO Calculate solution enthalpy of oxygen in titanium.

- The solution enthalpy E_{sol} and excess volume ΔV is

$$E_{\mathrm{sol}=E(\mathrm{Ti}_n\mathrm{O})-E(\mathrm{Ti}_n)-E(O)}$$

$$\Delta V = V(\mathrm{Ti}_n\mathrm{O}) - V(\mathrm{Ti}_n)$$

- $E(\mathrm{Ti}_n\mathrm{O})$ is the excess energ of the bulk supercell with n Ti atoms and one impurity atom. $E(\mathrm{Ti}_n)$ is the energy of the pure cells.

- Influence of cell sizes and solution enthalpy needs to be considered.

1.9 TODO Has anyone investigated the stacking faults of Omega phase?

- Maybe as Omega phase doesn't occur that often, perhaps it has not been studied in detail.

- I should look further into thsi

1.10 TODO Finish doing the gamma surfaces for all planes for pure titanium.

1.10.1 Checking the convergence criteria

- Now checking the convergence criteria.

1. How the lattice parameters change with the fineness of the k mesh

   - Maybe with a less fine k mesh the lattice parameters become worse.
   - SOLUTION: The lattice parameters do not change that much under

   differences with the k mesh. File with change of the lattice parameters with k mesh. a vs nk c_{vsnk} e_{vsnk}

   (a) What if rmaxh is smaller or larger?

   - If rmaxh is is smaller (say rmaxh = 6.7 bohr) then we get the same results.

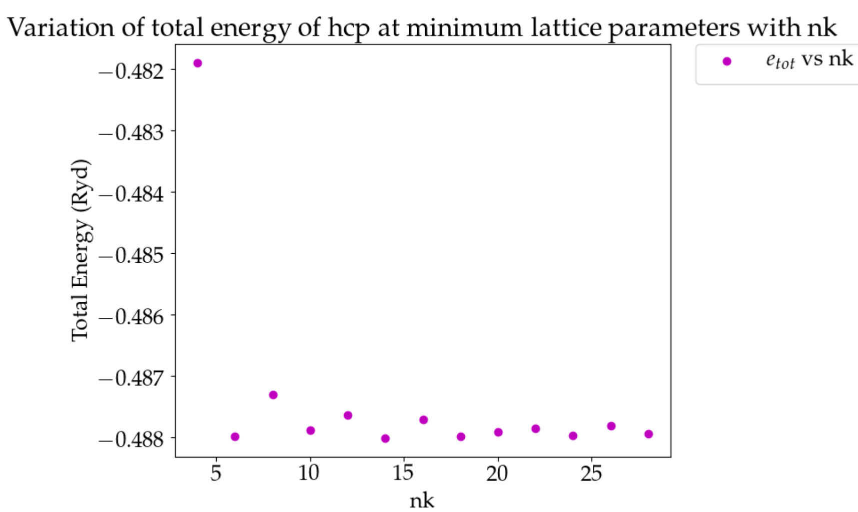


Figure 1: Variation of energy with k mesh.

]]

- Data: a_{hcp} small rmaxh, c_{hcp} small rmaxh, e_{hcp} small rmaxh.

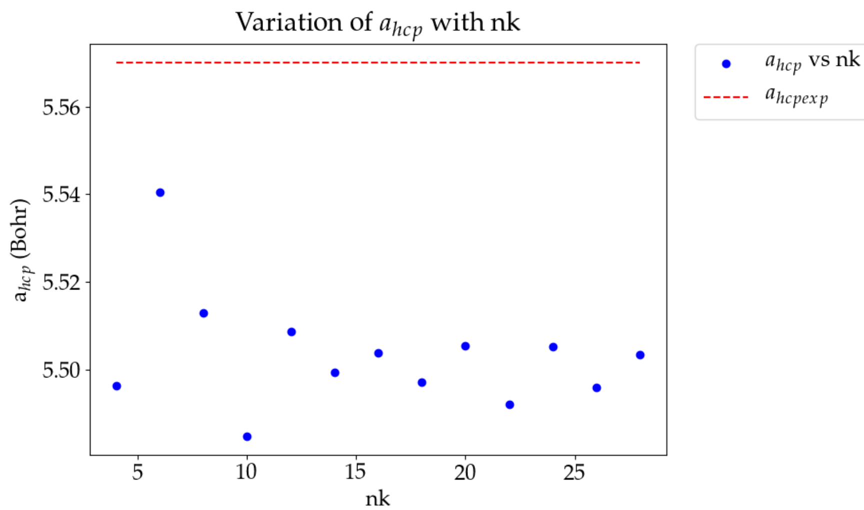


Figure 2: Variation of a hcp with k mesh.

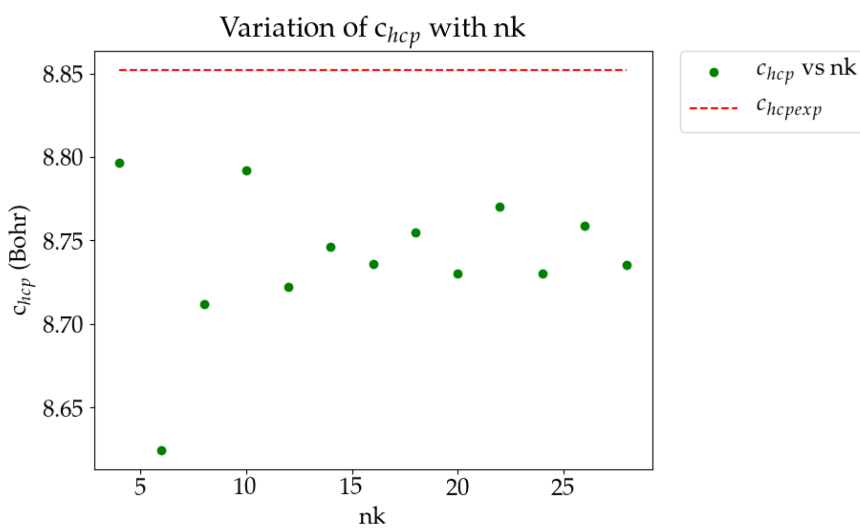


Figure 3: Variation of c hcp with k mesh.

- If rmaxh is larger (rmaxh = 20 bohr), all possible interactions must be included then. And so we get the same results.

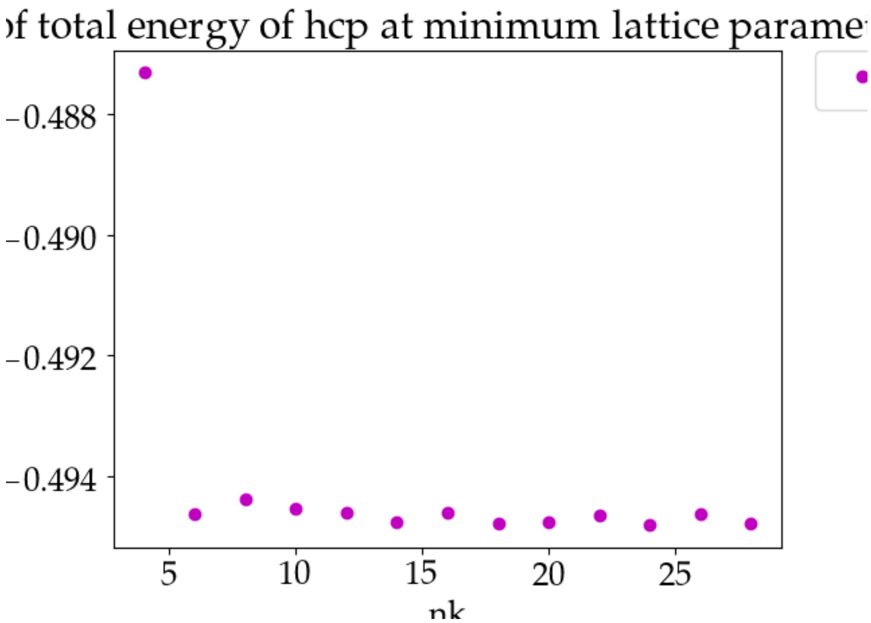


Figure 4: Variation of energy with k mesh.

- Data: a_{hcp} large rmaxh, c_{hcp} large rmaxh, e_{hcp} large rmaxh

2. How does rmaxh change the lattice parameters?

   (a) How does rmaxh change the energy of a supercell

   - How does the number of neighbours change and what is the relation between rmaxh and larger cell sizes.

1.10.2 Notes on the model.

It seems that there is a lot of charge moving around when doing the relaxations. I think that this may be due to the fact that there is no Hubbard U interactions, a parameter for the coulomb interaction, which stops the charges from moving freely.

- TBE control file is currently set to this:

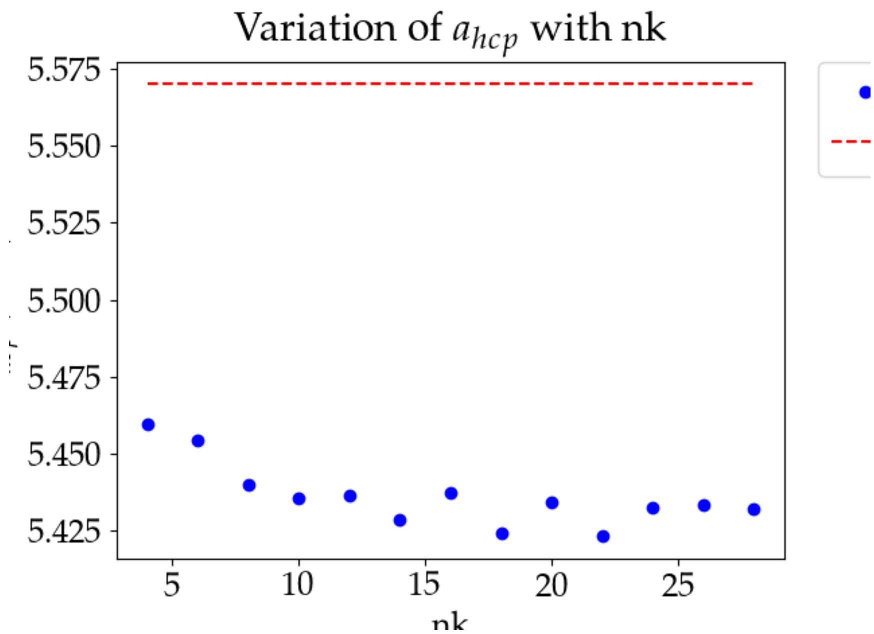


Figure 5: Variation of a hcp with k mesh.

1.10.3 DONE Implement Homogenous Shear boundary conditions for gamma surface calculation.

2 Notes

2.1 Dislocation dipole simulation

<2019-03-29 Fri> It seems that actually, for the Clouet method, the x component for the accomodaton of strain is *positive*. These additions to the tilt vectors make the dislocatons in a stable position in the quadrupolar array.

There is no asymmetry in relaxations now between the dislocations of different sign. This now works as expected.

2.2 Embedded atom method

This is a semi empirical method that does not take into account directional bonding. It does not treat covalency or charge transfer. Neither does it incorporate Fermi surface effects.

The main physical property incorporated in the EAM is the moderation

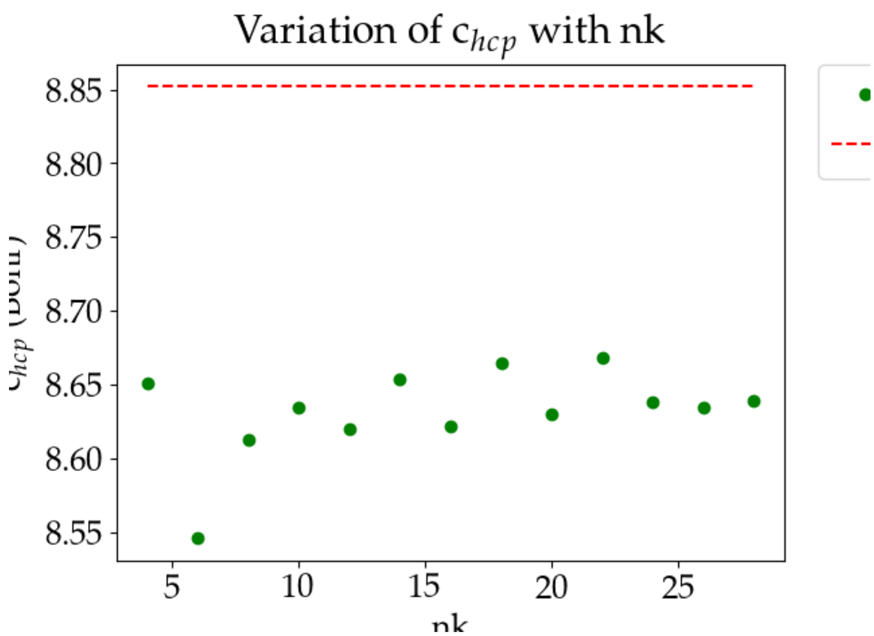


Figure 6: Variation of c hcp with k mesh.

of bond strength by other bonds (coordination-dependent bond strength).

3 Completed Tasks ARCHIVE

4 Bibliography

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[10] S. Banerjee, R. Tewari, and G. K. Dey. Omega phase transformation – morphologies and mechanisms. *International Journal of Materials Research*, 97(7):963–977, Jul 2006.

5 Current Papers

5.1 Omega phase transformation – morphologies and mechanisms.

Banerjee, S., Tewari, R., & Dey, G. K. (2006). International Journal of Materials Research, 97(7), 963–977. doi:10.3139/146.101327 [10]

Omega is found in both trigonal and perfect (hexagonal) forms.

Positions are: A: 0. 0. 0. B: 2/3 1/3 (1/2-z); 1/3 2/3 (1/2+z)

Where z = 1/6 is cubic symmetry.

The two atomic sites in the omega unit cell are not equivalent. B-type atomic sites are more closely packed as compare to the A-type atomic site.