Colour Map

If we have a property that is a function of more than one variable, we can represent this with a colour map.

Spin Transitions

Magnesiowüstite is one of the most abundant phase in the lower mantle. It has the chemical composition $Fe_{0.1}Mg_{0.9}O$.

Iron is a transition metal with unpaired d-electrons. In a crystal field, d-orbitals split and the electrons can arrange themselves into either a high-spin state, with four unpaired electrons, or a low-spin state, with all electrons paired. The state that the electrons adopt depends on the temperature and pressure.

Under pressure, it becomes more favourable for the electrons to form pairs, and a low-spin state forms.

You can estimate the fraction of iron in a low-spin state, denoted n, at any temperature and pressure from the expression

$$n(P,T) = \frac{1}{1 + m(2S+1)\exp\left[\frac{\Delta H_{LS-HS}(P)}{k_B X_{Fe} T}\right]}$$

where P is pressure, T temperature, m = 3 and is the orbital degeneracy of the high-spin state, S = 2 and is the total spin quantum number of the high-spin state, k_B is Boltzmann's constant, X_{Fe} is the fraction of iron in the phases and $\Delta H_{LS\text{-}HS}$ is the difference in enthalpy between the high- and low-spin states. Details of the derivation of this expression can be found in

> Tsuchiya et al. 2006. Spin Transition in Magnesiowüstite in Earth's Lower Mantle. *Phys. Rev. Lett.* **96**, 19850.

Initial Setup

The file *h.dat* contains the difference in enthalpy of the high- and low-spin states of ferropericlase with X_{Fe} = 0.1875 as a function of pressure. It is available from:

```
/nfs/ugrad-library/SOEE1160/practicals/practical_10
```

The first column is pressure in GPa and the second column is $\Delta H_{LS\text{-}HS}$ in eV.

Your Task

Your task is to write a MATLAB script that reads in the values from the file *h.dat,* calculates the value of $n(P,T)$ over a range of temperatures and pressures and plots them using the MATLAB function `pcolour`*.*

1. Use `fscanf` to read in the data from the file *h.dat.*
2. Use `polyfit` to fit a third-order polynomial to the values. To enable the estimate of $\Delta H_{LS\text{-}HS}$ at any pressure.
3. Use colon notation to create a vector containing the temperature values at which you want to calculate n (from 300 K to 4000 K).
4. Use colon notation to create a vector containing the pressure values at which you want to calculate n (from 1 GPa to 140 GPa).
5. Create a pair of nested `for` loops to loop over the temperature and pressure values, and calculate n at each one using the above equation (you will need to do some unit conversion, so that numerator and denominator of the fraction have the same units) and the third-order fit that you determined in 2.
6. Plot your values using `pcolour` and add a scale using `colourbar.` Use the MATLAB help, to find out how these work.
7. Try changing the temperature and pressure intervals used in Steps 3 and 4, smaller intervals will produce a more smooth plot.
8. You could also try adding the MATLAB statement `shading interp,` which causes values to be interpolated between data.

You should end up with something similar to: