

Assignment #3

Computational Material Thermodynamics

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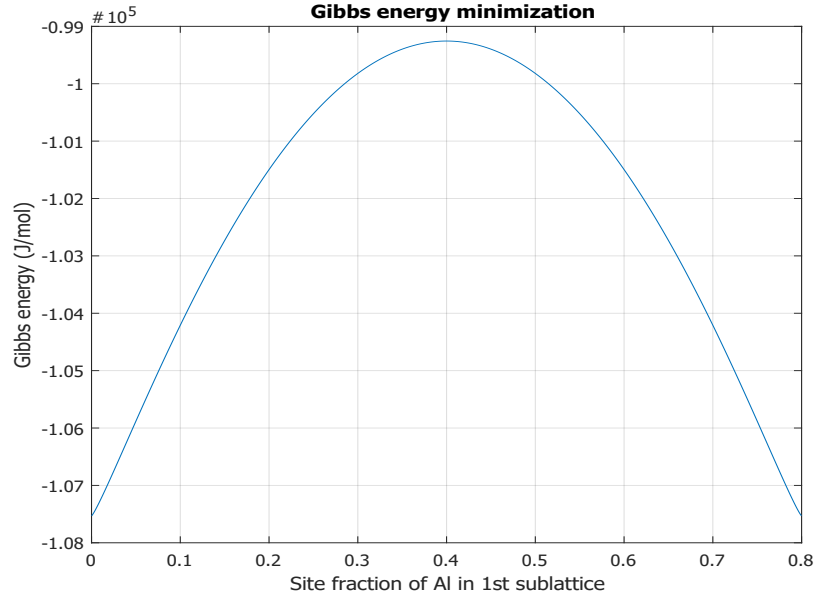


Figure 1: Gibbs energy vs $y_{Al\#1}$

$y_{Al\#1}$	0.7999	$y_{Al\#2}$	$5.2225e - 5$
$y_{Ni\#1}$	0.2001	$y_{Ni\#2}$	0.9999

Table 1: Minimisation of Gibbs Energy; $G_{min} = -1.0753e + 05 \text{ Jmol}^{-1}$

I used MATLAB scripts for summing up all contributions to Gibbs energy and plotting it while imposing the given constraints. No minima was observed and the lowest value was found at the start value. Scripts (*optimize_G_AlNi.m* and *G_AlNi.m*) can be found in the same directory as this report.