

## **Simulation Parameters File**

**name\_simulation\_parameters.txt:** contains all the parameters used in the simulation. It also contains the size of the crystal if the layer colouring routine is engaged.

This file contains all parameters input by the user into *CrystalGrower* for later reference. The structure of this file follows input.txt but also contains the additional data fed into *CrystalGrower* at runtime. All the questions asked by *CrystalGrower* are also listed next to the values input by the user making this a useful tool for checking previously run simulations.

If the simulation is run with layer colouring enabled, the final part of this file will contain the length of the crystal along the facets defined for colouring. E.g. if the (1,0,0) facet is selected for colouring, this file will contain the length of the crystal between the furthest point on the crystal in the (1,0,0) direction and the corresponding point on the (-1,0,0) facet (i.e. the crystal length in the *a* direction in nanometres). This information is listed for each simulation frame if the simulation was set to output multiple frames, meaning the size of the crystal can be plotted vs. the number of iterations.