**M6 MD Supo 1: Q2**

Q2.1

Ideal gas:

Chart

Description automatically generated

RDF constant with distance as expected; ideal gas has no potential energy/interactions so particles equally likely to be anywhere in system. Discrepancy at small distances where RDF is large?

Q2.2

Water O-O:

Chart, shape

Description automatically generated

Water O-H

Chart

Description automatically generated

Both RDF show liquid behaviour. Primary RDF peak at small distance corresponding to first coordination shell in water hydrogen bonded network. Very weak secondary RDF peak (especially subtle in O-O RDF) present corresponding to second coordination shell. No more peaks present because of fluxional liquid behaviour destroying position correlations for third nearest neighbours and greater.

2.3

Set 1

Chart

Description automatically generated

Set 2

Chart, histogram

Description automatically generated

Set 3

Chart, histogram

Description automatically generated

Set 1 is liquid phase (only two strong peaks before RDF decays). Sets 2 and 3 are crystalline (many peaks in RDF, showing that there is long-range order).

The coordination number corresponding to a crystalline peak in the RDF is given by:

This numerically approximates to

Where the sum is over all bins, i, corresponding to the crystalline peak and is the bin width.

For set 2: Looking at first three peaks in more detail. Judge minima by eye (marked as red circles).

Table

Description automatically generated

Coordination no. for first three peaks are 0.0143, 0.0208 and 0.0239 respectively. These numbers are too small so likely a normalisation error during RDF calculation (perhaps I wasn’t meant to divide by no of atom pairs?). However, can still work out ratios of coordination numbers relative to first peak as approximately 1, 1.5 and 1.7 for the respective peak.

Use this table of data to identify crystalline phase based off coordination number ratio of peaks.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Crystal structure | 1st nearest neighbours | 2nd nearest neighbours | 3rd nearest neighbours | Expected ratio pattern |
| Fcc | 12 | 6 | 24 | 1, 0.5, 3 |
| Bcc | 8 | 6 | 12 | 1, 0.75, 2 |
| Hcp | 12 | 6 |  | 1, 0.5, |
|  |  |  |  |  |

Set 1 does not correspond to any of these crystal structures. No. of bins should be increased to give more accurate values (I used N\_bins = 100).

For set 3:

Chart, line chart

Description automatically generated

Table, Excel

Description automatically generated

Again, ratio pattern 1, 1.25, 1.48 doesn’t match any of the crystal structures in the table. Conclusion: no. of bins too small to get an accurate value of coordination number.