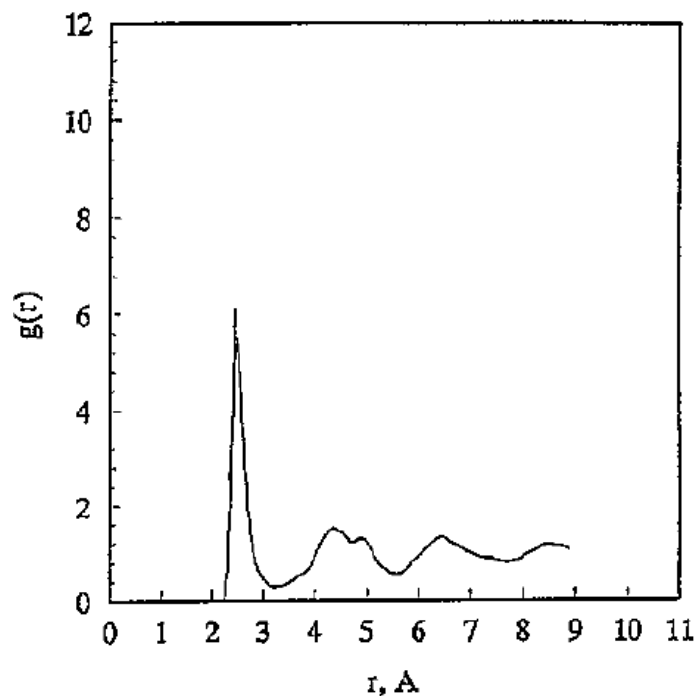


Interpretation of RDF and material identification

RDF



- (a) Explain if this is a solid, liquid, or gas. Justify your answer briefly.
- (b) What do the peaks mean? Explain the meaning of the first three peaks **from the left**.
- (c) Which of the below shown materials is the one shown in the RDF? Explain briefly why.

1. Bulk copper ☐
2. Carbon nanotube ☐
3. Liquid argon ☐
4. Liquid nickel ☐

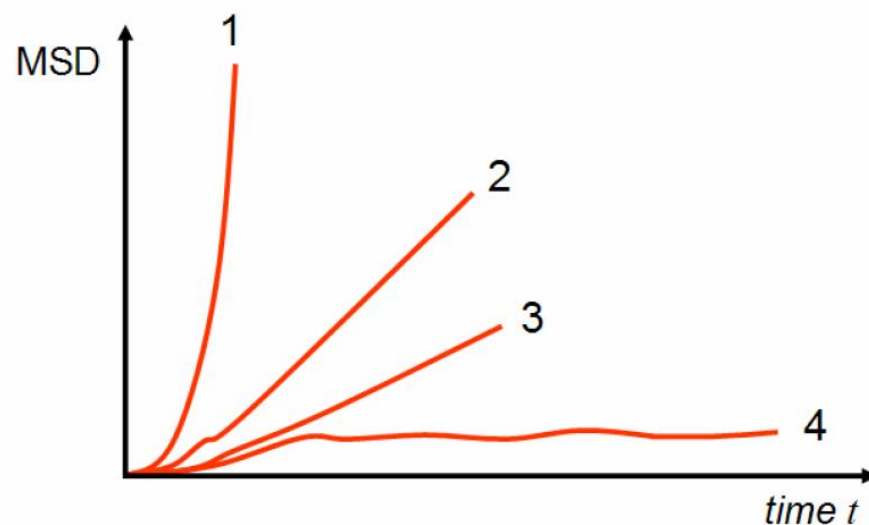
Analysis of molecular dynamics simulation runs

In the list below, mark those properties for which you need dynamical information of your system (that is, more than one snapshot in time):

1. Radial distribution function (RDF) ☐
2. Mean square displacement function (MSD) ☐
3. Temperature ☐

Mean Squared Displacement function

For the graphs shown below, indicate which one is a liquid, gas or solid.



For the liquids identified above, indicate in the graph how you can determine the diffusion constant D

Solution can be done graphically, sketch sufficient.

Lecture 5 - questions

1. Explain the definition and interpretation of the Radial Distribution Function (RDF). What type of information can you extract?
 2. Using the RDF, can you distinguish between a metal and a polymer?
 3. What is particular about the RDF of water? Would that hold for other materials (give examples)?
 4. Describe the different types of chemical bonds.
 5. Describe the parameters in the LJ potential. What are the limitations?
-
6. Were the goals of today's lecture clear?
 7. Was today's lecture clear?
 8. Did you feel that today's lecture contributed to your understanding of the topic?
 9. What could have been improved in order to make this lecture more useful?