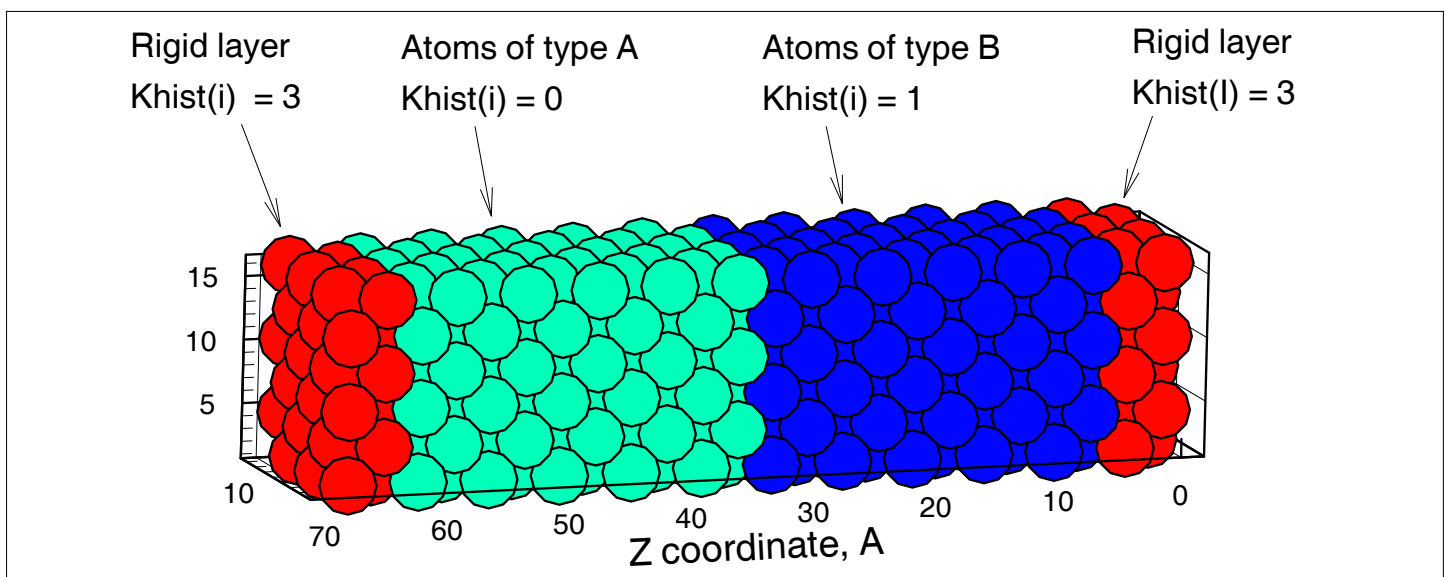


## Homework #5 (page 1 of 2)

**Objective:** Understanding the relation between microscopic mechanisms and continuum description of diffusion.

1. Using the same FCC crystal that you used in homework #3 (5x5x5 unit cells, 500 atoms,  $a_{\text{fcc}} = 5.78 \text{ \AA}$ ), perform two simulations, one below the melting temperature  $T_m$ , another at  $T = 1.5T_m$ . Use the value of  $T_m$  that you found in homework #3, not the experimental one. Run the simulations for a time sufficient to collect data for the calculation of the diffusion coefficient.
2. Using Einstein relation calculate the diffusion coefficient,  $D$ , for the two temperatures. Attach plots that are used in the calculations.
3. Pick a few (2-3) particles and plot their trajectories (e.g. a projection of the trajectory to a 2D plane plotted for a time equal to several periods of atomic vibrations) for the same two simulations as in task #1. Discuss, relate to the plots and values of  $D$  that you calculated in task #2.
4. Perform simulation study of self-diffusion for a system shown at the bottom of the this page (use input file *ArDiff.data* from ...mse627/MSE627-MD/hw4). This file has 3x3x12 FCC unit cells (432 atoms), lattice constant  $a_{\text{fcc}}$  is 5.78  $\text{\AA}$ . Size of the computational cell is 17.32 $\text{\AA}$ ×17.32 $\text{\AA}$ ×69.36 $\text{\AA}$ . (continued at the next page)



## Homework #5 (page 2 of 2)

Variable KHIST(I) is used to define rigid atoms (KHIST(I)=3), atoms of type A (KHIST(I)=0), and atoms of type B (KHIST(I)=1). All atoms are interacting among each other via the same interatomic potential (KTYPE(I)=1 for all atoms). You can think about atoms of type B as isotopes of atoms of type A. Thus, in this simulation you will study self-diffusion of Ar.

Choose parameters in md.input so that you have periodic boundary conditions in X and Y directions, and rigid boundaries in Z directions.

In this simulation use the highest of the two temperatures used in task #1. Use your knowledge of D (from task #2) to estimate the time of the simulation that would give you a significant mixing of atoms A and B. Explain your choice of the total time of the simulation. Also, use your knowledge of D to estimate an appropriate value for input parameter NPER (that defines how often you have to gather molecules to the original computational cell). Explain your choice of NPER.

Plot snapshots of your system (mark atoms A and B in a different way) and concentration profiles for atoms of type B for three different times during the simulation.

**5. (optional for undergraduates)** Perform continuum calculation of the evolution of the concentration profiles by solving the diffusion equation. Use the same size of the computational cell as in MD simulation (task #4) and the value for diffusion coefficient that you found in task #2. Run the simulation for the same time as the MD simulation. Compare the concentration profiles obtained in the continuum and MD simulations, discuss the observed agreement/disagreement.

**This is your last homework!**  
**Happy computing and good luck with your term projects!**