Dave Juergens

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NetLogo Simulation – Things to try

1. Estimate the temperatures at which atoms are solid, liquid, gas phase
   1. Starting with 917 atoms, 0.19 density, and HCP packing. The lattice remains solid until ~ T=0.45-0.5. Somewhere around here the phase changes.
   2. I lose the ability to detect the difference between the liquid and gas phases at about T = 1-1.1. So at this point, the system transitions from a liquid to a gas phase. At t > 1.1 the system remains gaseous.

1. When starting without an HCP configuration, are you able to return to the HCP when lowering the temperature?
   1. Yes! This was super cool actually (lol literally and figuratively). I started with a random initial configuration with 917 atoms, density = 0.25, and initial temperature at 1.1. At this point the atoms were very evenly dispersed in a semi-gaseous phase. I slowly “annealed” the configuration, dropping the temperature gradually. By the time I dropped the temperature to 0.01, I achieved various HCP nucleation sites in the volume.
   2. Why? Well, as temperature drops, the atoms have less freedom to explore. The lowest energy state they can adopt is to be a (certain) close distance away from each other. When the atoms have less kinetic energy, they are unable to remove themselves from the potential energy well at this distance, and thus adopt a packing scheme allowing for as many atoms as possible to be in this favorable state.
2. What is the lowest energy per particle state? Why is the lowest energy this value?
   1. I’m unable to find a consistent absolute lowest value for energy per particle. However, what I do notice is that whenever a given simulation starts in HCP phase, this is the lowest energy-per-particle state accessible. When the HCP lattice is heated up into a gaseous phase by adding temperature, and then you take away the exact same amount of temperature, you do not return to the same energy per particle you had before. This is because the system does not return to a perfect HCP lattice, but instead various HCP nucleation sites. Because this is not a perfect HCP lattice, it is in a higher energy state than the initial configuration at the same temperature.
3. When starting with less atoms, does the temperature at which phase changes occur change? Why or why not?
   1. I would say yes. When starting with 14 atoms, density = 0.25, HCP lattice, the phase has already turned liquid by T = 0.3. By T = 0.8, the phase is surely gaseous. I think this is because in a large lattice, the cumulative effect of many LJ potentials tends to draw atoms inward with more force, so it’s harder for atoms in a larger lattice to break free. In a small lattice, there is less of this cumulative effect.