

# Questions about MD simulations of polycrystalline copper

March 18, 2014

1. In the material sample of copper I am doing simulations on(I'm using molecular dynamics package LAMMPS), I use centrosymmetry parameter to visualize grain boundaries, slip planes etc. Is it optimal to do so, or is there a better way to do it? I am using a program named Ovito to do it. Also I am having a difficulty with locating the grain boundaries based only on centrosymmetry(pictures of the system are at the end of the file, with centrosymmetry parameter depicted with rainbow style color gradient). How I could visualize them, meaning how could I really tell there is a clear-cut grain boundary?
2. More on grain boundaries - if in the material sample I am using grain boundaries are not very well defined and there is a lot of rubbish, how can I make them appear better? Heat the material? If so, for how long and at what temperature? Would simulation time of 0.1 ns (order of magnitude) be enough? Should the temperature be something really close to the melting temperature of copper?
3. One problems seems to be, that the example is already compressed to a high extent, how can I make sure from the centrosymmetry picture, that no plastic deformation has taken place? If there has been, how can I return the material to a elastic state? Also with heating?
4. If I wanted to create my own sample of polycrystalline copper from a monocrystalline copper sample, how should I do it? Could it be done with melting and cooling? Is it feasible with MD? How could I control the size of grains created in my sample?
5. General questions about MD simulations - if I'm using periodic boundary conditions (my box size exactly encompasses the extent of atoms) with a npt ensemble, essentially simulating a bulk material I have to set the temperature and pressure at the "boundaries". I am a little confused how this works, because if my system is periodic and extends to all space, where is the boundary? I could understand the case when my system wouldn't be periodic and there would be, for example a heat bath/sink connected to one side of my simulation box, likewise for pressure.

Figure 1: whole sample

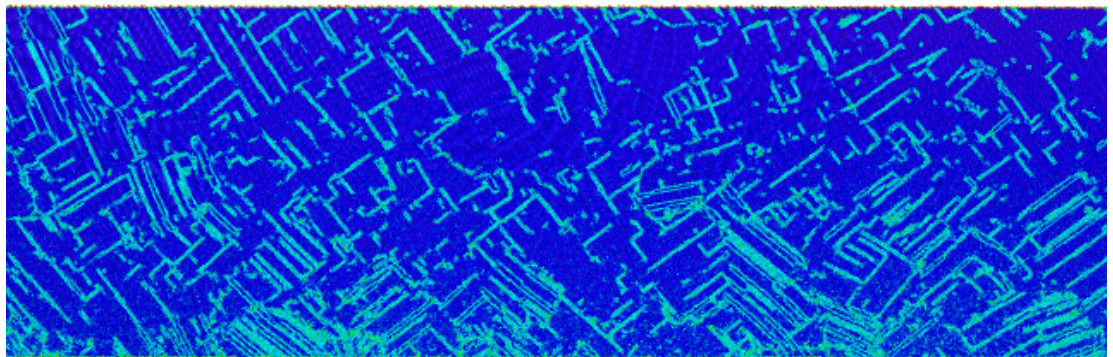


Figure 2: perspective view

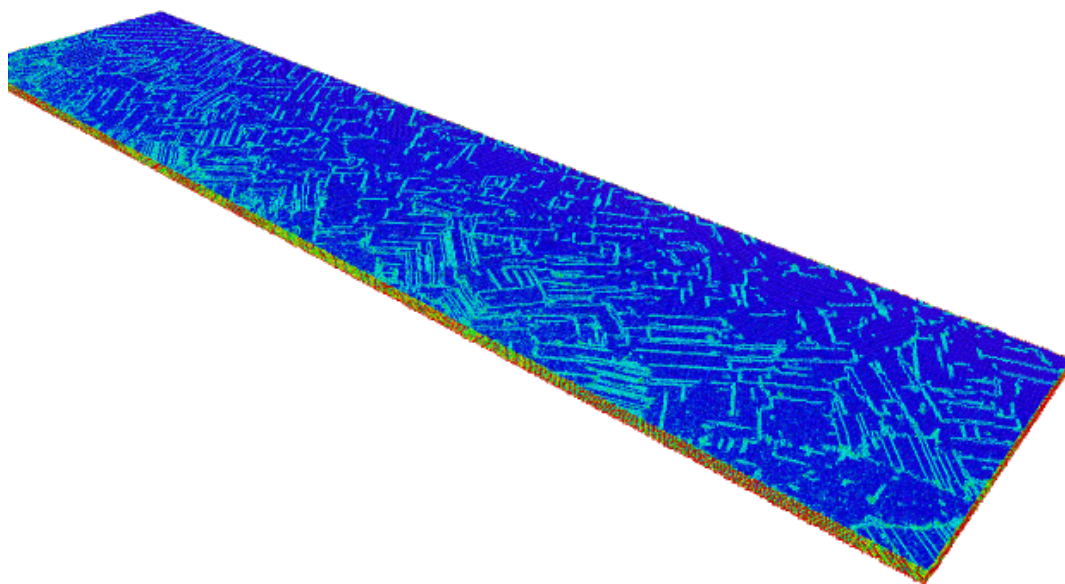


Figure 3: closer look 1

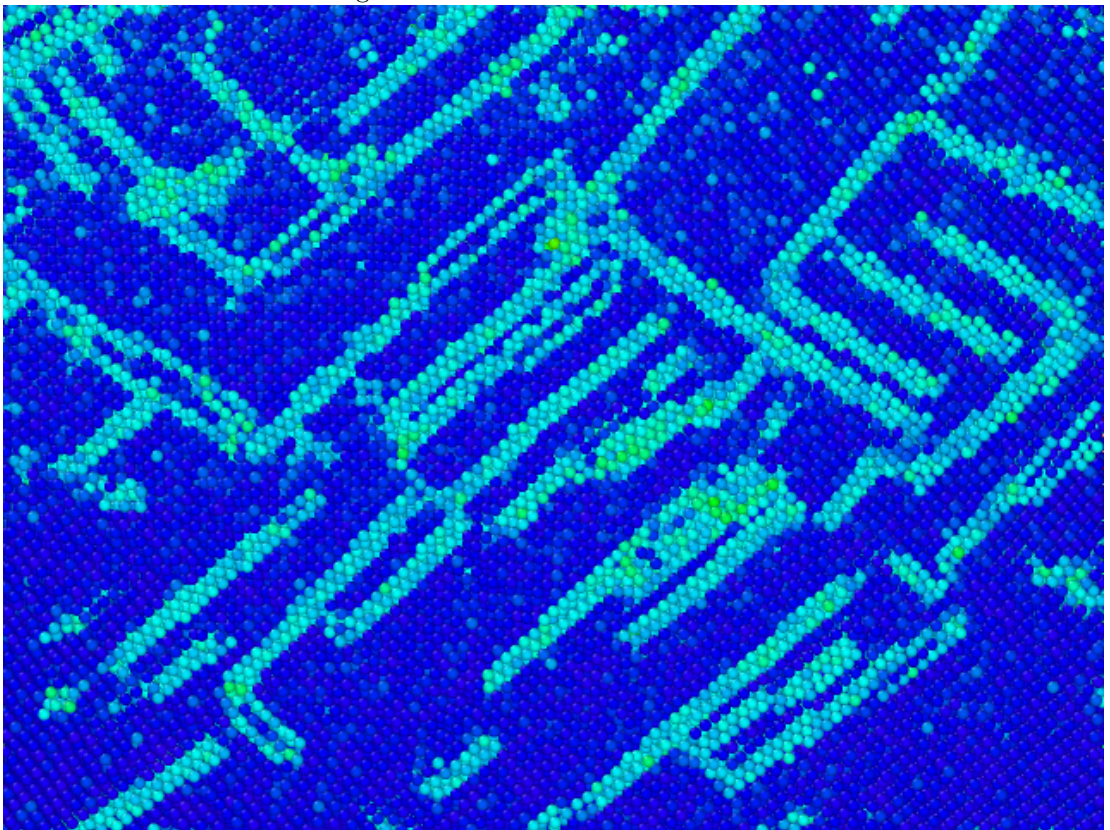




Figure 4: closer look 2

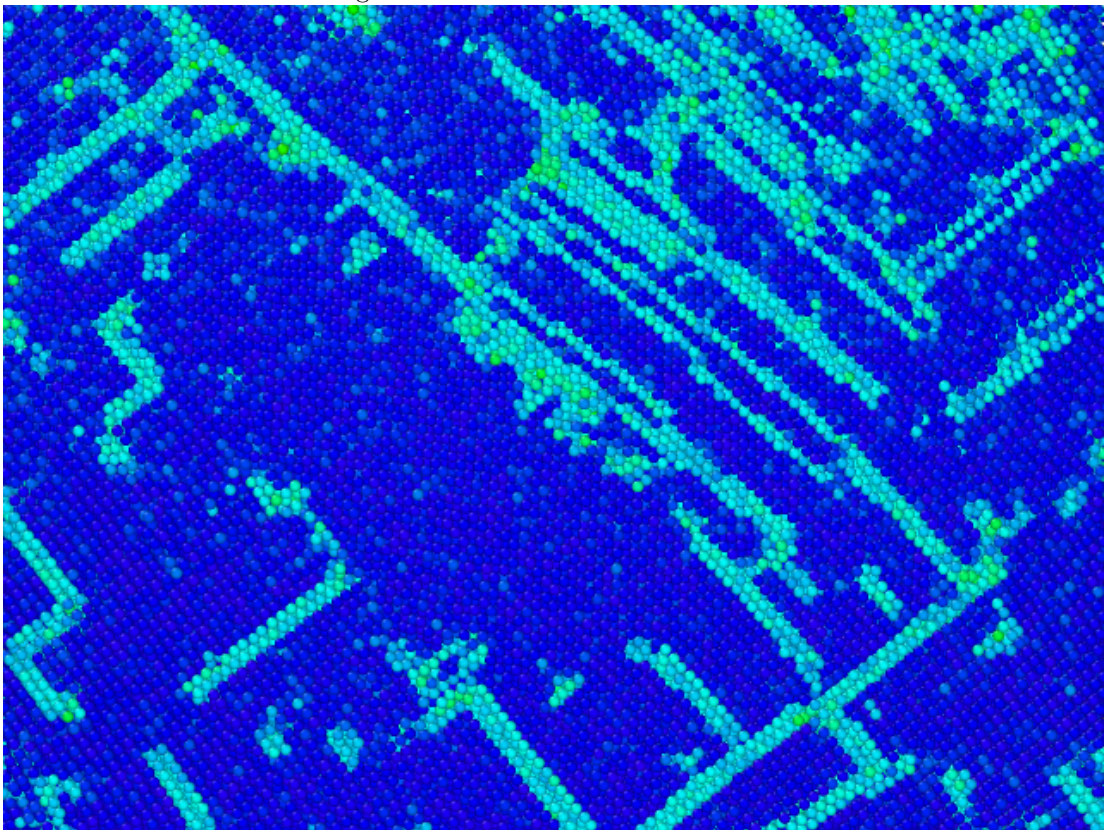


Figure 5: closer look 3

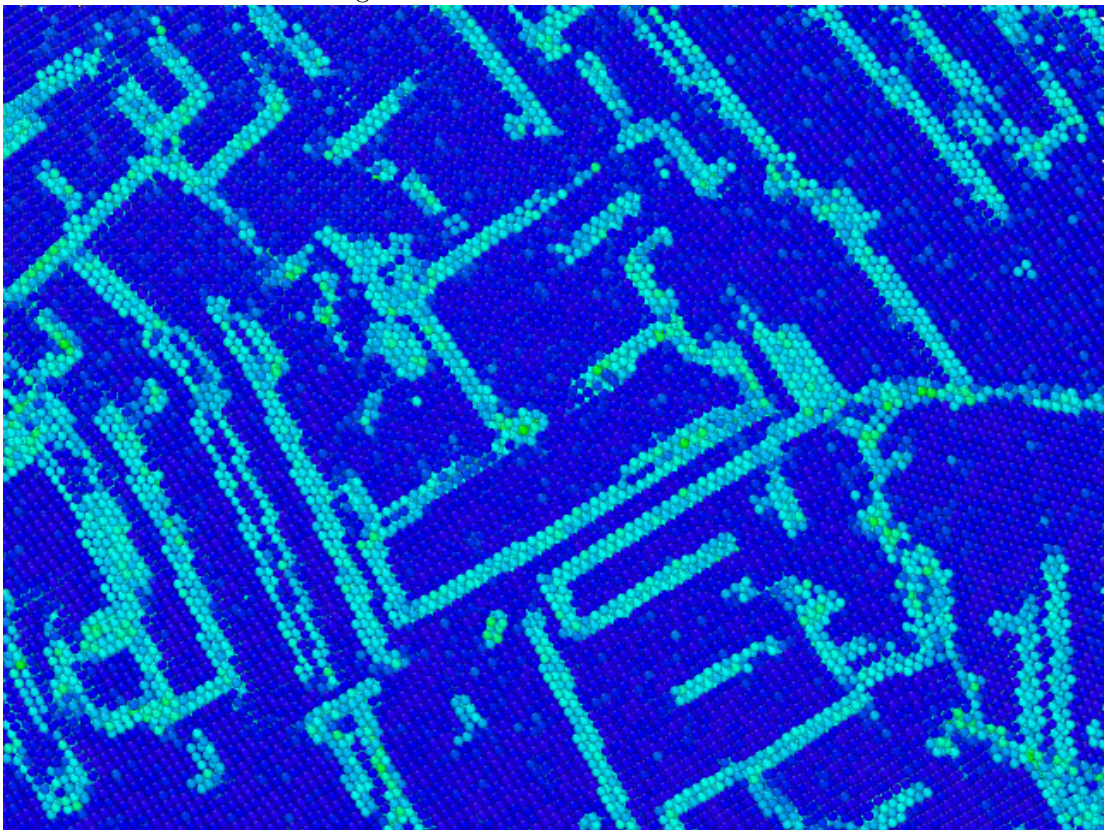
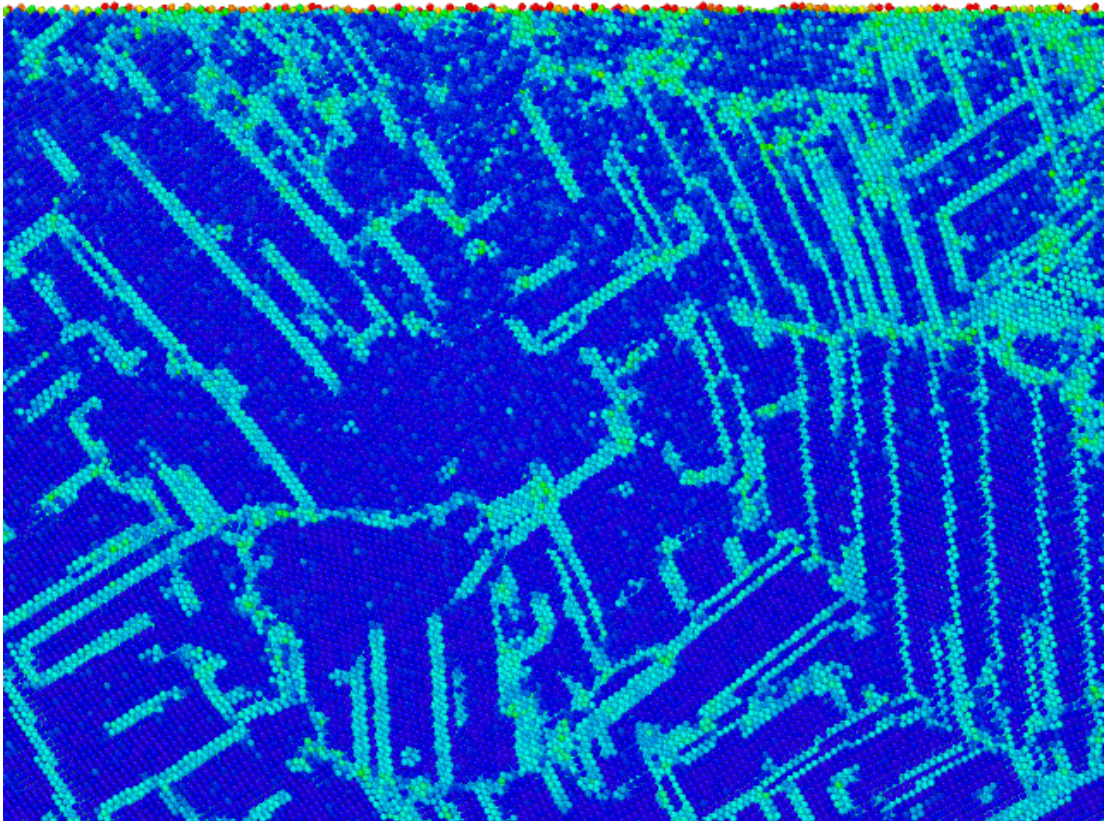




Figure 6: closer look 4





## Simulation details

Here I enlist the details of one of my simulations I am doing on a material sample I created from the thin plate I depict in the pictures. I am trying to heat up a sample representing a bulk material, in order to see, if the structure of grains becomes more vivid. (pilt).

- about 3.1 million atoms
- periodic boundary conditions in all directions
- timestep 1 fs
- potential file Mishin *et al*
- npt ensemble with barostat and thermostat, set at 1340K and 0.0 Pa, with pressure and temperature damping parameters both 0.1. I also couple all of the diagonal components of the stress tensor  $P_{xx}, P_{yy}, P_{zz}$  together.

Do these choices make sense? On what basis should I choose a good temperature and pressure damping parameter while using Nose-Hoover thermostat and barostat? While equilibrating one of my other simulations with the same setup and parameters at 800K, my pressure fluctuations(one third of the sum of the diagonal components) had an maximum amplitude of 200 bars ( $200 * 10^5$  Pa). Is it normal or problematic? The individual components varied by about 1400 bars.

Figure 7: setup created from the thin plate. Simulation box boundaries are in black.

