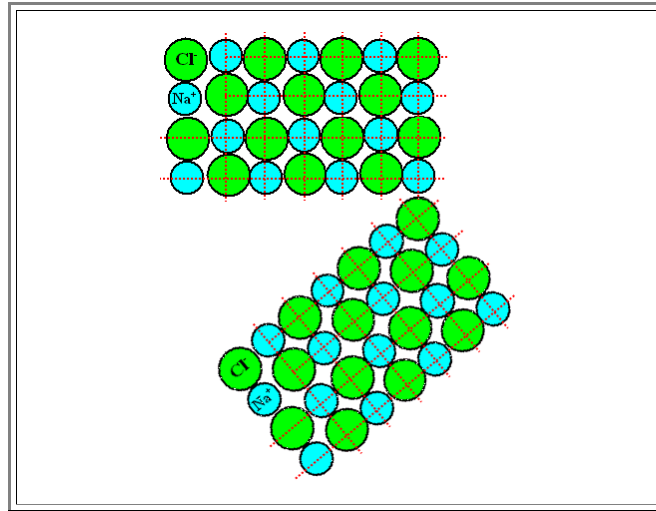


Exercise: Make a Grain Boundary in Salt

Let's look at a grain boundary in a simple crystal like sodium chloride (NaCl) known as common salt. Take the two grains shown below that are only rotated with respect to each other and join them, producing a grain boundary viewed "edge-on"

The atoms here are charged, they are actually ions. The big green atoms symbolize negatively charged chlorine, the blue atoms positively charged sodium. Since unlike charges attract each other and like charges oppose each other, the rules for filling in ions are

- Green atoms must only touch blue atoms and vice versa.
- There should be an equal number of blue and green atoms because there is no net charge.
- Atoms should be closely packed.



Can you do it? I can't. That's why there is no link to a solution.

- The crystal, however, has no problem to come up with an arrangement of atoms that produces a nice switch-over from one grain to another one. Not just for the geometry shown here but for *any* possible geometry.
- To *compute* the atomic structure, however, is hellishly difficult.