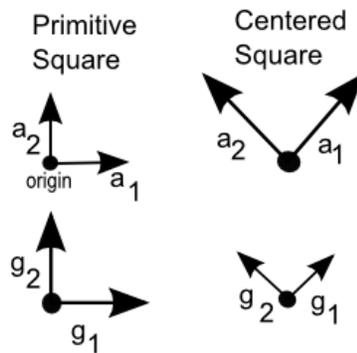


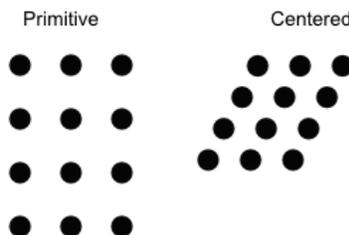
Topic 3-5: Centered Lattices

**Summary:** In this video we discuss centered lattices in reciprocal space. We find that, just as with real space vectors, a primitive and centered square cell create the same space when the structure factor is accounted for.

- When we construct real space lattices the vectors and origins we choose are rather arbitrary
  - Let's see what the consequence is on reciprocal space when we vary our choice of real space lattice. We'll do this in 2D to make the visualization easier, but this is exactly the same in 3D
- In real space a centered square cell does not reveal anything new about the lattice



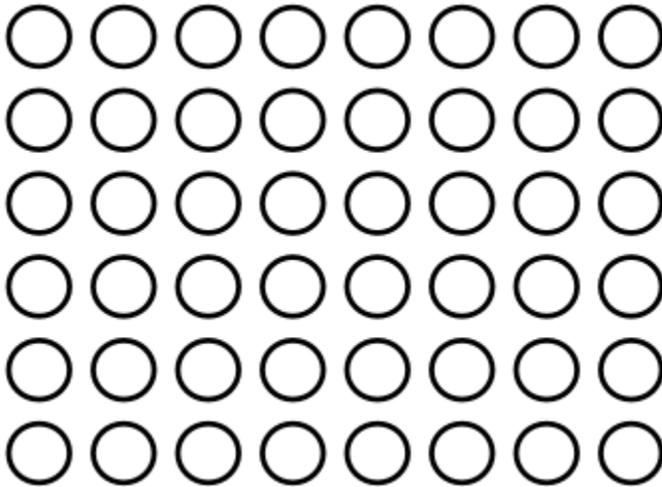
- The magnitude of  $a_1$  of the primitive cell is *less* than the magnitude of  $a_1$  in the centered square cell. Thus, the magnitude of  $g_1$  of the primitive cell will be *greater* than the magnitude of  $g_1$  of the centered cell.
- Populating space with these reciprocal lattices we get



- Initially, this looks really bad. However, this is practically okay as long as the intensity works out the same.

- Let's put an arsenic atom at each lattice point (basis:  $As = (0,0)$ ). For the primitive cell we find (in video 3-3) the structure factor  $S=f_0$  for all  $h, k$  (note 2D now) and there were peaks at every lattice point
- For the centered cell we found  $S=2f_0$  for  $h + k = \text{an even integer}$  while  $S=0$  for  $h + k + 1 = \text{an odd integer}$ , which puts peaks at every other lattice point

Show that the above bullet actually works out visually



- This gives equal spacing of expected peaks even though the lattice points originally look different
- Centering and unit cell selection therefore makes no difference when it comes to diffraction; the choice will ultimately be accommodated in the structure factor.

Questions to Ponder

1. If we start with a square lattice in real space but pick primitive oblique lattice vectors do we still get a square lattice in reciprocal space?