Problem set due on November 8, **before** the beginning of the lecture

1 Bravais lattices in two dimensions: reciprocal space (10 points)

Here we want to continue the work on Bravais lattices begun in the last exercise of the previous assignment. The same crystal structures are shown in Fig. 1.

a) For the crystal structures which you have previously identified as Bravais lattices, calculate the corresponding primitive unit vectors of the reciprocal lattice (Hint: since this is 2D, you cannot use the definition given in the lecture which contains a cross product and is thus inherently 3D; however, the relation $\mathbf{a}_i\mathbf{b}_j = 2\pi\delta_{ij}$ is still valid...).

b) Sketch how the reciprocal lattice will look like in each case.

c) Construct (i.e. draw) the first Brillouin zone, i.e. the Wigner-Seitz cell of the reciprocal lattice you sketched in b).

2 Close packing of spheres (12 points)

A guiding principle in the formation of crystals is often to fill the available space as efficiently as possible. Here we want to study the "space filling" in different three-dimensional Bravais lattices. Consider crystals consisting of touching hard spheres with a radius r. Calculate the fraction of the volume which is filled (i.e. which lies inside one of the hard spheres) compared to the total volume of the crystal for the following cases:

(i) A primitive cubic lattice; (ii) A body-centered cubic lattice and (iii) A face-centered cubic lattice.

Hints: imagine having point-like "spheres" at first and let them expand until they touch their nearest neighbors... what is their volume? What is the volume of a primitive unit cell in each particular lattice type? Since we are only interested in the *ratio* between sphere volume and total volume, you don't need to use absolute numbers for the calculation. You can relate lengths to an arbitrary coordinate system, as for example indicated in Fig. 2: Since $|\mathbf{a}_1| = |\mathbf{a}_2| = |\mathbf{a}_3| = a$, the primitive unit cell volume is a^3. Now place the hard spheres at the lattice positions... what is their volume in terms of a? For the more complicated lattices in (ii) and (iii), the primitive vectors will not necessarily be perpendicular – in the lecture it was shown how to calculate the primitive unit cell volume in this case. Alternatively, you could also work with the conventional cubic unit cell, but then you must keep in mind that you will have more than one atom (sphere) per such unit cell.

Finally, determine the coordination number for the three lattices. Do you see a qualitative relation to the filling ratios?

(iv) Gain 4 extra points for calculating the filling ratio and coordination number of the diamond lattice (look it up on the web). Can you imagine why nature chooses the diamond structure with a low the filling ratio for diamond, while in metals or ionic crystals, lattices with high filling ratios are found, such as body- or face-centered lattices?

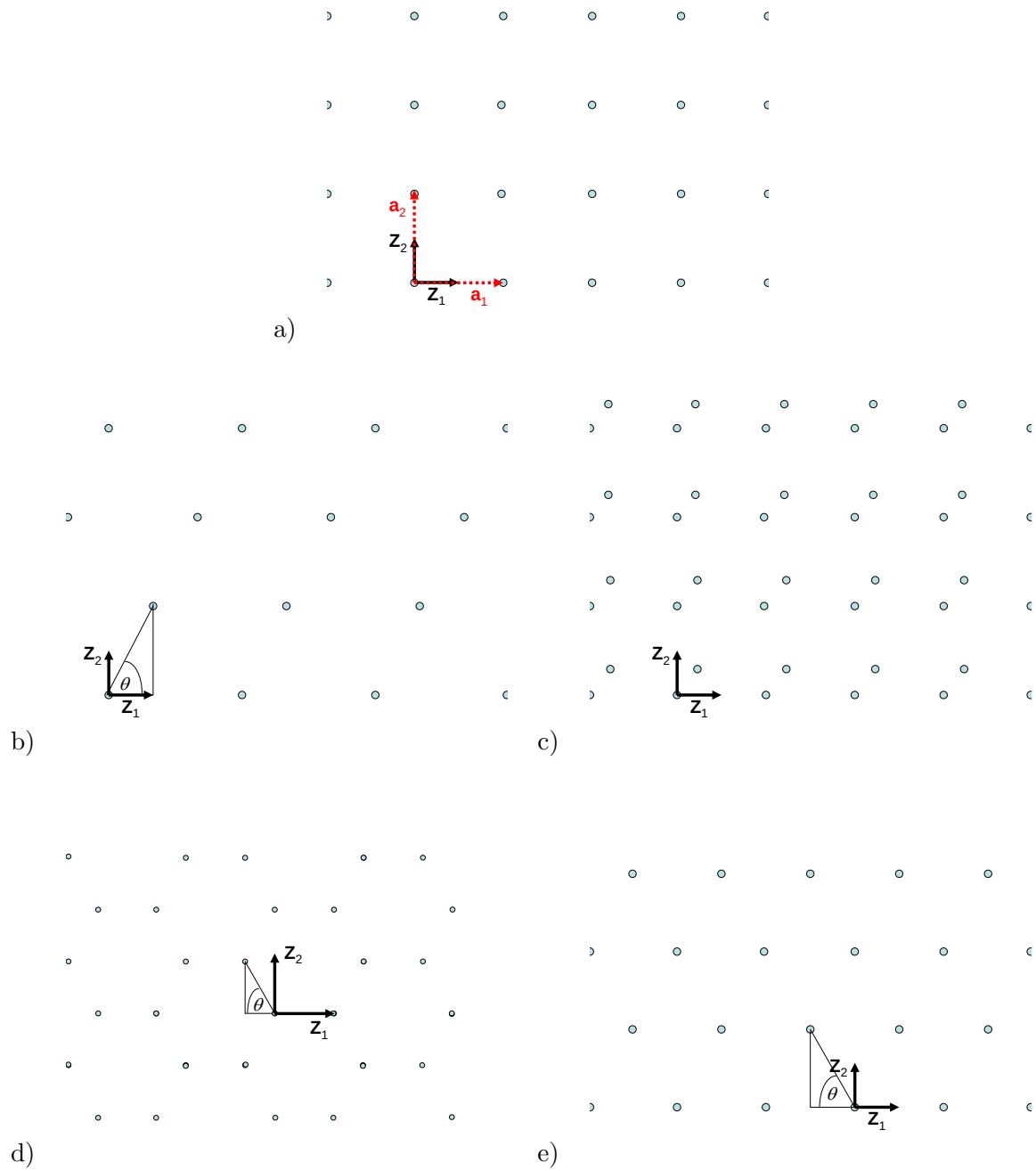

Figure 1: Different two-dimensional lattices. Panel a) shows a square Bravais lattice; a set of possible primitive vectors is defined by $\mathbf{a}_1 = 2\mathbf{z}_1$ and $\mathbf{a}_2 = 2\mathbf{z}_2$. In b), $\tan\theta = 2$, and in d) and e), $\theta = 60°$.

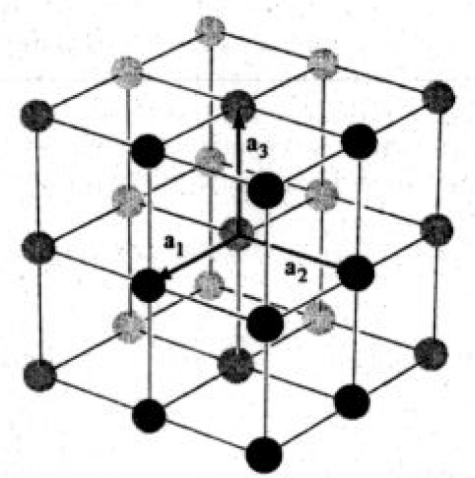

Figure 2: Simple cubic lattice with a particular choice of a coordinate system, for which the primitive unit vectors coincide with the unit vectors of the coordinate system.