MSE 102, Fall 2018 Problem Set #1
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(1) Lattice terminology. The structure on the next page displays a portion of a lattice. (As you know, a lattice is infinite in extent.) The blue points represent the lattice points. These points can all be written as

$$\mathbf{R}_{uv} = u\,\mathbf{a} + v\,\mathbf{b},$$

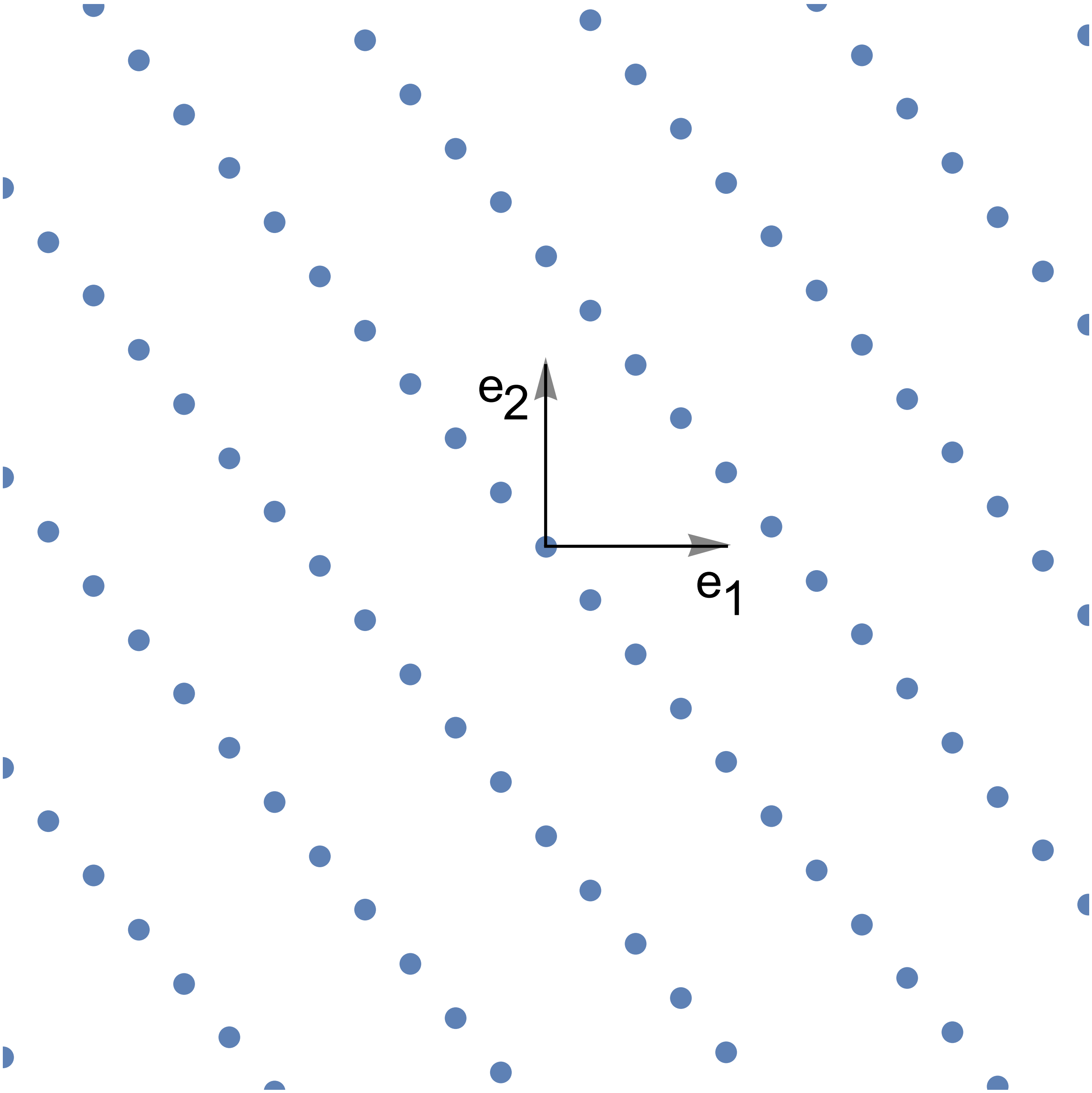
with

$$\mathbf{a} = -\frac{3}{4}\,\boldsymbol{e}_1 - \frac{1}{\sqrt{2}}\,\boldsymbol{e}_2$$

$$\mathbf{b} = 1\,\boldsymbol{e}_1 + \frac{1}{\sqrt{6}}\,\boldsymbol{e}_2,$$

and $\mathbf{e}_1$ and $\mathbf{e}_2$ are the unit vectors in the x and y directions, respectively. The vectors $\mathbf{a}$ and $\mathbf{b}$ are known as primitive lattice vectors, because from them, you can generate every lattice point in the structure. In the plot, I show the unit vectors drawn to scale.

- [5 points] Sketch the primitive lattice vectors on the plot.
- [5 points] The primitive lattice vectors are not unique. To prove this, identify another set of primitive lattice vectors that also describe the same lattice.
- [10 points] Construct the Wigner-Seitz primitive cell for this lattice. You can do this by hand if you like – sketching the procedure on the figure.
- [5 points] Identify a lattice point as 00. Then identify the $\left[2\,\overline{3}\right]$ direction for each set of primitive lattice vectors.
- [5 points] Indicate the $\overline{3}1$ point for both sets of primitive lattice vectors.



e2
e1

(2) [10 points] Along which line do the planes (111) and $(1\bar{1}1)$ intersect? (Use the zonal equation.)

(3) [10 points] Give the Miller indices of the plane is defined by the two directions $[111]$ and $[2\bar{1}3]$.

(4) A 3D lattice is defined by the primitive lattice vectors:

$$\boldsymbol{a} = \frac{1}{2}\,\boldsymbol{e}_2 + \frac{1}{2}\,\boldsymbol{e}_3$$

$$\boldsymbol{b} = \frac{1}{2}\,\boldsymbol{e}_1 + \frac{1}{2}\,\boldsymbol{e}_3$$

$$\boldsymbol{c} = \frac{1}{2}\,\boldsymbol{e}_1 + \frac{1}{2}\,\boldsymbol{e}_2\ .$$

Here, the vectors $\boldsymbol{e}_1$, $\boldsymbol{e}_2$, and $\boldsymbol{e}_3$ are unit vectors in the x-, y- and z- directions, respectively.

[10 points] Sketch, to the best of your abilities, a portion of the lattice, and draw the primitive lattice vectors on the sketch.

[15 points] Sketch the structure of the (111) plane. (That is, plot the lattice points that appear within a single (111) plane in a 2D plot with the view normal to the lattice plane.)

[15 points] Sketch the structure of a (110) plane. (That is, plot the lattice points that appear within a single (110) plane in a 2D plot with the view normal to the lattice plane.)

(5) [10 points] The Materials Project (https://materialsproject.org) is a database of computed properties for materials, including a large number of crystalline solids. This database was started by Profs. Persson and Ceder, and has grown into a wonderful tool to explore the properties of known and hypothetical materials. I will try and make use of this site throughout the course. So, for your assignment, sign up to use the Materials Project at the link given above. Conduct a search for compounds containing only Ti and Nb. One of these will have the symmetry Pm3m (space group 21). What are the computed lengths of the lattice vectors used to describe this structure? What is the predicted volume per conventional unit cell for this structure?