Utrecht University
Exam Solids and Surfaces
Tuesday, February 1st, 2022
Time: 13:30 - 16:30

Name and student number: _____

Good luck!

- Write your name on each answer sheet.
- Answer Q1 and Q2 on separate sheets of paper.
- Please pay attention to your hand-writing. If we cannot read your answers, we cannot award points.
- In your answers, do not immediately start with equations. Also draw conclusions from the calculations you have done.
- Preferably answer in English.
- Please note that you can earn a maximum of 35 points.
- Not each question is worth the same number of points.
- The following relations might be helpful:

$$\cos(2a) = 2\cos^2 a - 1$$
$$\cos(a+b) + \cos(a-b) = 2\cos(a)\cos(b)$$
$$\cos(a+b) = \cos(a)\cos(b) - \sin(a)\sin(b)$$
$$\cos(a-b) = \cos(a)\cos(b) + \sin(a)\sin(b)$$
$$e^{ik} + e^{-ik} = 2\cos(k)$$
$$\sin(x) \approx x \text{ (for small } x)$$

Question 1: **Geometric structure of surfaces** ..... *11 points*

(a) (3 points) Copper has an FCC crystal structure. The surface energy of the Cu(111) surface is 0.67 eV/(surface atom). Compute the surface energy of the Cu(100) **AND** Cu(110) surfaces.

(b) (2 points) Arrange these copper surfaces in the order of ascending work function. Explain.

(c) (4 points) Determine the equilibrium shape of a Cu crystal using the {111}, {110} and {100} planes. Use $\gamma_{100} = 1$ eV and $\gamma_{110} = 2$ eV. **IMPORTANT:** These values do *not* correspond to the answers to question 1a. It is not essential that your drawings are exactly to scale.

(d) (2 points) Name two surface preparation techniques that can be used to prepare this atomically flat and clean surface.

Question 2: **Tight Binding calculations** ..... *24 points*

Consider the crystal shown in Fig. 1. The black circles indicate the positions of the atoms. In this question, you will perform a tight-binding calculation of this structure. Each atom contributes one electron and one s-type orbital. Only interactions with nearest neighbors have to be taken into account.

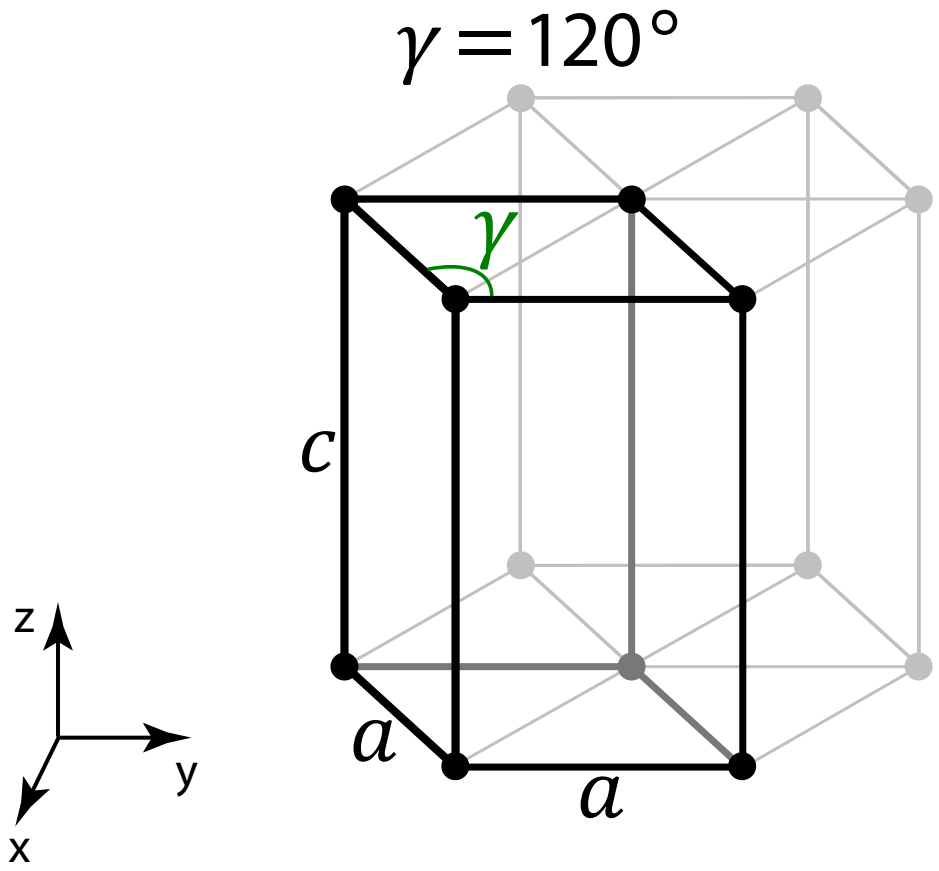

Figure 1: Hexagonal lattice. Note the orientation of the spatial directions x, y and z.

(a) (3 points) Determine the primitive unit cell vectors using the directions indicated in Fig. 1. Set $c = a$.

(b) (4 points) Based on your previous answer, determine the primitive unit cell vectors of the reciprocal lattice.

(c) (9 points) Show that the dispersion relation of this material can be written as

$$E(\boldsymbol{k}) = \epsilon + 2t\cos(k_y a) + 4t\cos(k_y a/2)\cos(k_x\sqrt{3}a/2) + 2t\cos(k_z a) \qquad (1)$$

(d) (3 points) A large force is applied along the z-axis that pulls the atomic planes apart. Does this change the band structure? Explain.

(e) (2 points) Do you expect this material to be a metal, semi-conductor, or insulator? Explain.

(f) (3 points) Assume that you want to make your calculation more accurate by including a second s-type orbital with a significantly higher on-site energy for each atom. Describe how this will change the calculation and the results (is it still a metal or not?) You do not need to do the calculation.