Utrecht University
Exam Solids and Surfaces
Tuesday, January 29th, 2019
Time: 13:30 - 16:30

Name and student number: ____________________

Good luck!

- Write your name on each answer sheet.
- 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.
- You can answer in English or in Dutch.
- Please note that you can earn a maximum of 73 points.
- Not each question is worth the same number of points.
- The following relations might be helpful:

$$\begin{aligned}
\cos(2a) &= 2\cos^2 a - 1 \\
\cos(a+b) + \cos(a-b) &= 2\cos(a)\cos(b) \\
\cos(a+b) &= \cos(a)\cos(b) - \sin(a)\sin(b) \\
\cos(a-b) &= \cos(a)\cos(b) + \sin(a)\sin(b) \\
e^{ik} + e^{-ik} &= 2\cos(k)
\end{aligned}$$

Question 1: **Metal surface** . . . . *24 points*

(a) (4 points) Suppose you want to do experiments on a Cu(111) surface. Which method would you use to prepare an atomically flat and clean surface Cu(111) surface? Explain.

(b) (2 points) The crystal structure of Cu is fcc. Sketch how the atoms in the top-layer are arranged.

(c) (4 points) Indicate the $[1\bar{1}0]$ and $[22\bar{1}]$ directions in your sketch.

(d) (4 points) Creating a surface costs energy. How does the surface energy of a Cu(111) surface *quantitatively* compare to that of a Cu(100) and Cu(110) surface? Explain.

(e) (2 points) The Cu(111) surface features an electronic state localized at the surface. What is the physical origin of this state?

(f) (3 points) Sketch the wave function of the surface state in the direction perpendicular to the surface.

(g) (5 points) Describe the approach to calculate the surface state wave function for a semi-finite 1D chain of atoms. You do not have to do the calculation itself, just describe which steps you have to take.

Question 2: **The 2D triangular lattice** . . . . *49 points*

Consider the 2D triangular lattice with nearest neighbor distance a shown in Figure 1. One choice of lattice vectors is

$$\boldsymbol{a_1} = \frac{a}{2}\hat{x} + \frac{\sqrt{3}a}{2}\hat{y} \tag{1}$$

$$\boldsymbol{a_2} = \frac{a}{2}\hat{x} - \frac{\sqrt{3}a}{2}\hat{y} \tag{2}$$

In this question, you will perform a tight-binding calculation of this structure. Only interactions with nearest neighbors have to be taken into account. Each atom contributes one s orbital and one electron.

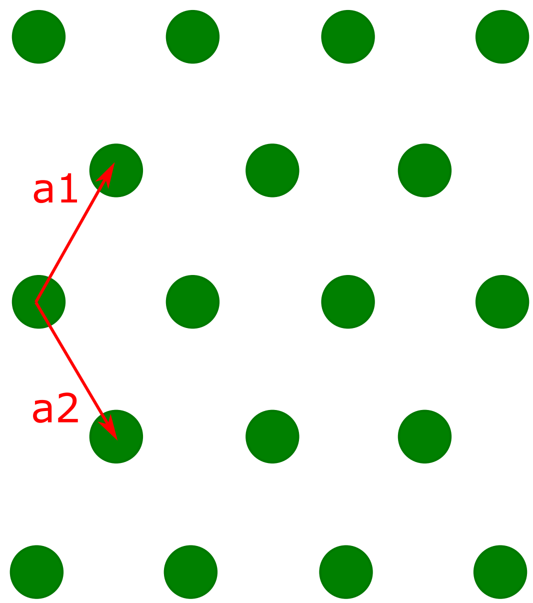

Figure 1: 2D triangular lattice. Note the $\hat{x}$ and $\hat{y}$ directions and lattice vectors.

(a) (3 points) Draw the Wigner-Seitz cell of the lattice shown in Figure 1, include the different steps used to arrive at your answer.

(b) (7 points) Determine the reciprocal space lattice vectors **AND** draw the reciprocal space lattice and lattice vectors.

(c) (2 points) What is the name of the Wigner-Seitz cell in reciprocal space?

(d) (3 points) How many terms do you expect in the expression for the expectation value of the energy? Explain.

(e) (11 points) Show that a nearest-neighbor tight-binding calculation results in the following dispersion relation.

$$E(\boldsymbol{k}) = \alpha - 2\beta + 4\beta \cos\left(\frac{a}{2}k_x\right)\left[\cos\left(\frac{\sqrt{3}a}{2}k_y\right) + \cos\left(\frac{a}{2}k_x\right)\right] \tag{3}$$

(f) (4 points) Given the dispersion relation, explain if this material is a metal, semiconductor or insulator. Include the term *Fermi level* in your answer.

(g) (8 points) Typically, the band structure is plotted along the high symmetry directions of the reciprocal space unit cell. Starting from equation (3), sketch the dispersion relation along the following three lines:

- from the center of the unit cell (Γ) to one of the corners of the cell (K, located at $\left(\frac{4\pi}{3a}, 0\right)$)
- from the corner mentioned above to the M-point, located at $\left(\frac{\pi}{a}, \frac{\pi}{\sqrt{3}a}\right)$
- from the M-point back to the Γ-point.

Take care of the values of the energy. You can set $\alpha = 0$ eV.

(h) (1 point) Given your assignment in question *1f* (metal, semiconductor, insulator), explain if scanning tunneling microscopy (STM) and spectroscopy (STS) experiments can be performed on this material.

(i) (6 points) Assume that one can perform STS experiments on this material. Given the dispersion relation, equation 3, sketch the differential conductance spectrum that one would expect.

(j) (4 points) Sketch the Low Energy Electron Diffraction pattern that one would see for a clean 2D triangular surface.