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:

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

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.

Answer: Cu is a relatively noble metal. A clean surface is therefore most easily obtained by removing the contaminants via sputtering and annealing (2 points). Creating a flat surface by cleaving is impossible because of the isotropic bond strengths in all directions (1 point). Epitaxial growth may work, depending on the lattice constant of substrate on which the film is grown (1 point).

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

Answer: The atoms in a Cu(111) surface are close-packed. The arrangement is sketched in Figure 1 (2 points).

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

Answer: $[1\bar{1}0]$ corresponds to the close-packed direction, $[22\bar{1}]$ perpendicular to it (2 points for each correct answer).

(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.

Answer: The Cu(111) surface is the most densely packed and therefore the most stable (1 points). Quantitative statements can be made via the broken-bond-ratio. 3,4, and 6 bonds need to be broken per surface Cu atom to create a Cu(111), Cu(100) and Cu(110) surface, respectively. Hence, it costs approximately $4/3 = 1.33$ and $6/3 = 2$ times as much energry to create a Cu(100) and Cu(110) surface, respectively.

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

Answer: The surface breaks the periodicity of the crystal (1 point). This allows additional solutions to the Schrödinger equation (1 point).

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

Answer: See Figure 3.9a of the reader. There is an exponentially damped wave inside the crystal (2 points), matched by an exponentially decaying function outside the crystal (1 point).

(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.

Answer: The minimum model required for surface states is the nearly-free electron model, where the periodic potential generated by the ion cores is represented by a function that has the same periodicity as the lattice (1 point). The surface is modeled by a potential step (1 point). You take a trial solution of the wave function of the form $\psi(x) = \sum_G c_G e^{i(k-G)x}$, with c_G constants (1 point). It is in principle sufficient to take only the first two terms. Finally, you solve the Scrödinger equation for the two regions separately (1 point) and use the boundary conditions to determine the full wave function (1 point).

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

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

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

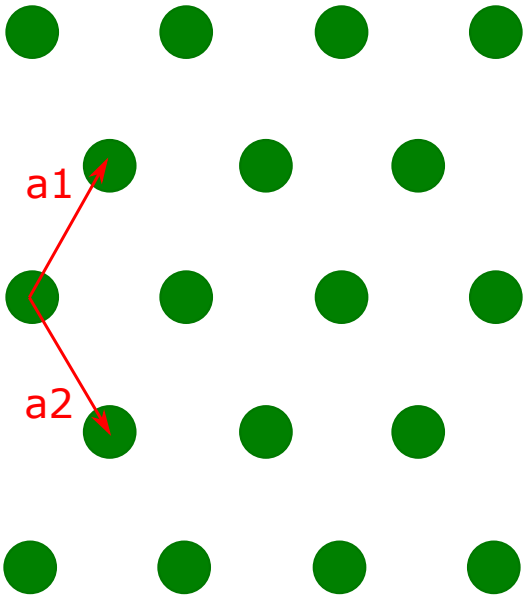

Figure 1: 2D triangular lattice. Note the $\hat{x}$ and $\hat{y}$ directions and lattice vectors.

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.

(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.

Answer: The WS cell is indicated by the light-green hexagon in the figure below. 1 point for the correct drawing, 2 points for using the correct procedure.

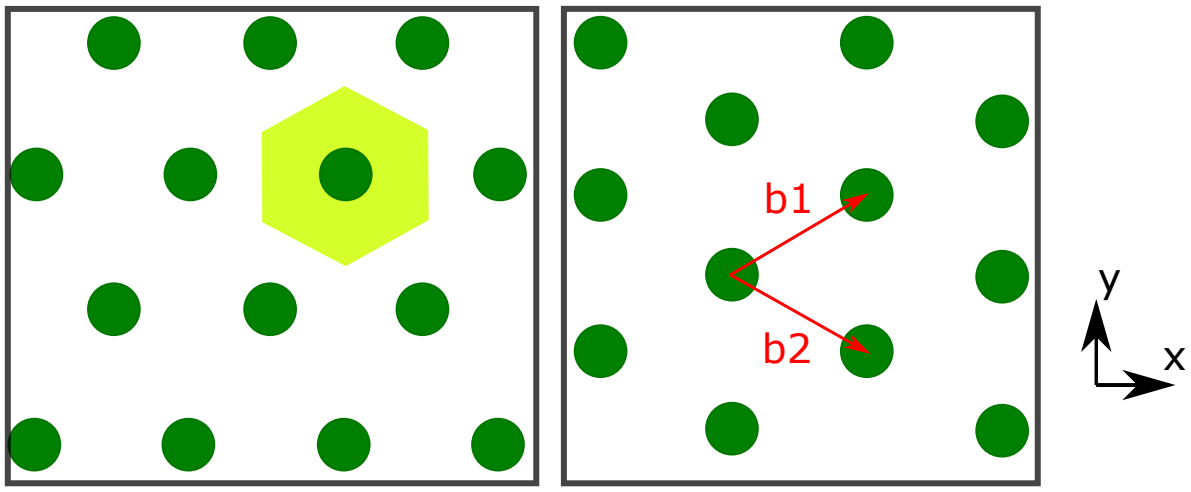

Figure 2: Left: 2D triangular lattice with Wigner-Seitz cell indicated. Right: reciprocal space lattice and corresponding lattice vectors.

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

Answer: Use the relation $\boldsymbol{b_i} \cdot \boldsymbol{a_j} = 2\pi\delta_{i,j}$ (1 point) to find

$$\boldsymbol{b_1} = \frac{2\pi}{a}\hat{x} + \frac{2\pi}{\sqrt{3}a}\hat{y} \tag{3}$$

$$\boldsymbol{b_2} = \frac{2\pi}{a}\hat{x} - \frac{2\pi}{\sqrt{3}a}\hat{y} \tag{4}$$

(2 points for each correct answer). From this, it is clear that the reciprocal lattice of a 2D triangular lattice is also a 2D triangular lattice (2 points for the correct drawing, including orientation). Note the rotation w.r.t. Figure 1.

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

Answer: Brillouin zone (2 points).

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

Answer: 7 (1 point), 1 on-site term, and 6 for the interactions between nearest neighbors (2 points).

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

$$E(\boldsymbol{k}) = \alpha - 2\beta + 4\beta \cos\left(\frac{a}{2}k_x\right)\left[\cos\left(\frac{\sqrt{3}a}{2}k_y\right) + \cos\left(\frac{a}{2}k_x\right)\right] \tag{5}$$

Answer: Evaluate the expectation value of the energy (3 points),

$$E(\boldsymbol{k}) = \sum_{\boldsymbol{R}} e^{i(\boldsymbol{R}-\boldsymbol{R'})\boldsymbol{k}} \int \psi_{\boldsymbol{R'}} |\hat{H}| \psi_{\boldsymbol{R}}\, \boldsymbol{dr} \tag{6}$$

There are 7 terms

$$E(\boldsymbol{k}) = \alpha + \beta e^{i\boldsymbol{k}\boldsymbol{a_1}} + \beta e^{i\boldsymbol{k}\boldsymbol{a_2}} + \beta e^{-i\boldsymbol{k}\boldsymbol{a_1}} + \beta e^{-i\boldsymbol{k}\boldsymbol{a_2}} + \beta e^{i\boldsymbol{k}(\boldsymbol{a_1}+\boldsymbol{a_2})} + \beta e^{-i\boldsymbol{k}(\boldsymbol{a_1}+\boldsymbol{a_2})} \tag{7}$$

3 points for the correct expression. Using the definitions of the primitive lattice vectors, (a_i), this can be written as

$$E(\boldsymbol{k}) = \alpha + \beta[e^{i(ak_x/2+\sqrt{3}ak_y/2)} + e^{i(ak_x/2-\sqrt{3}ak_y/2)} + e^{-i(ak_x/2+\sqrt{3}ak_y/2)} + e^{-i(ak_x/2-\sqrt{3}ak_y/2)} + e^{iak_x} + e^{-iak_x}] \tag{8}$$

2 points. Use $e^{ix} + e^{-ix} = 2\cos(x)$ to find

$$E(\boldsymbol{k}) = \alpha + 2\beta\left[\cos\left(\frac{a}{2}k_x + \frac{\sqrt{3}a}{2}k_y\right) + \cos\left(\frac{a}{2}k_x - \frac{\sqrt{3}a}{2}k_y\right) + \cos\left(ak_x\right)\right] \tag{9}$$

$$= \alpha + 2\beta\left[2\cos\left(\frac{a}{2}k_x\right)\cos\left(\frac{\sqrt{3}a}{2}k_y\right) + \cos\left(ak_x\right)\right] \tag{10}$$

$$= \alpha - 2\beta + 4\beta\cos\left(\frac{a}{2}k_x\right)\left[\cos\left(\frac{\sqrt{3}a}{2}k_x\right) + \cos\left(\frac{a}{2}k_x\right)\right] \tag{11}$$

Here, we made use of $\cos(a+b)+\cos(a-b) = 2\cos(a)\cos(b)$ and $\cos(2a) = 2\cos^2 a - 1$. 3 points for the correct answer.

(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.

Answer: Each atom contributes 1 electron and 1 orbital. Hence, the band given by equation (5) is half full, i.e. the Fermi level is located in the middle of the band (2 points). Since there are empty states immediately above the Fermi level, a material with a 2D triangular lattice would be a metal (2 points).

(g) (8 points) Typically, the band structure is plotted along the high symmetry directions of the reciprocal space unit cell. Starting from equation (5), 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.

Answer: 2 points for each correct line (including correct values).

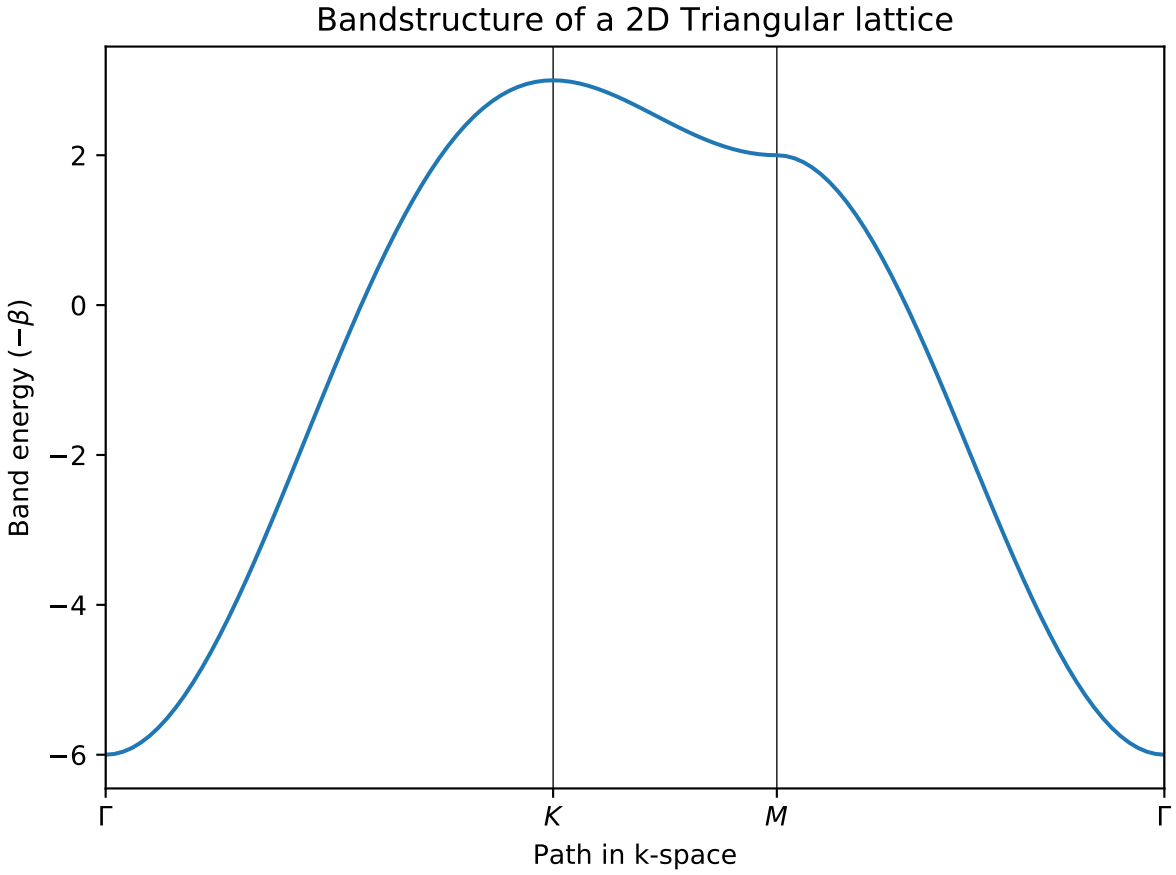

Figure 3: band structure of the 2D triangular lattice.

(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.

Answer: Since the 2D triangular lattice with one orbital and one electron per site is a metal, STM/STS experiments should be possible (1 point).

(i) (6 points) Assume that one can perform STS experiments on this material. Given the dispersion relation, equation 5, sketch the differential conductance spectrum that one would expect.

Answer: The differential conductance spectrum is proportional to the density of states (2 points). The DOS is the number of states per unit energy, integrated over all $\boldsymbol{k}$-values. Flat regions in the band structure, e.g. around the M-point, have a large DOS, which decreases to zero for the top (K) and bottom (Γ) of the band (2 points).

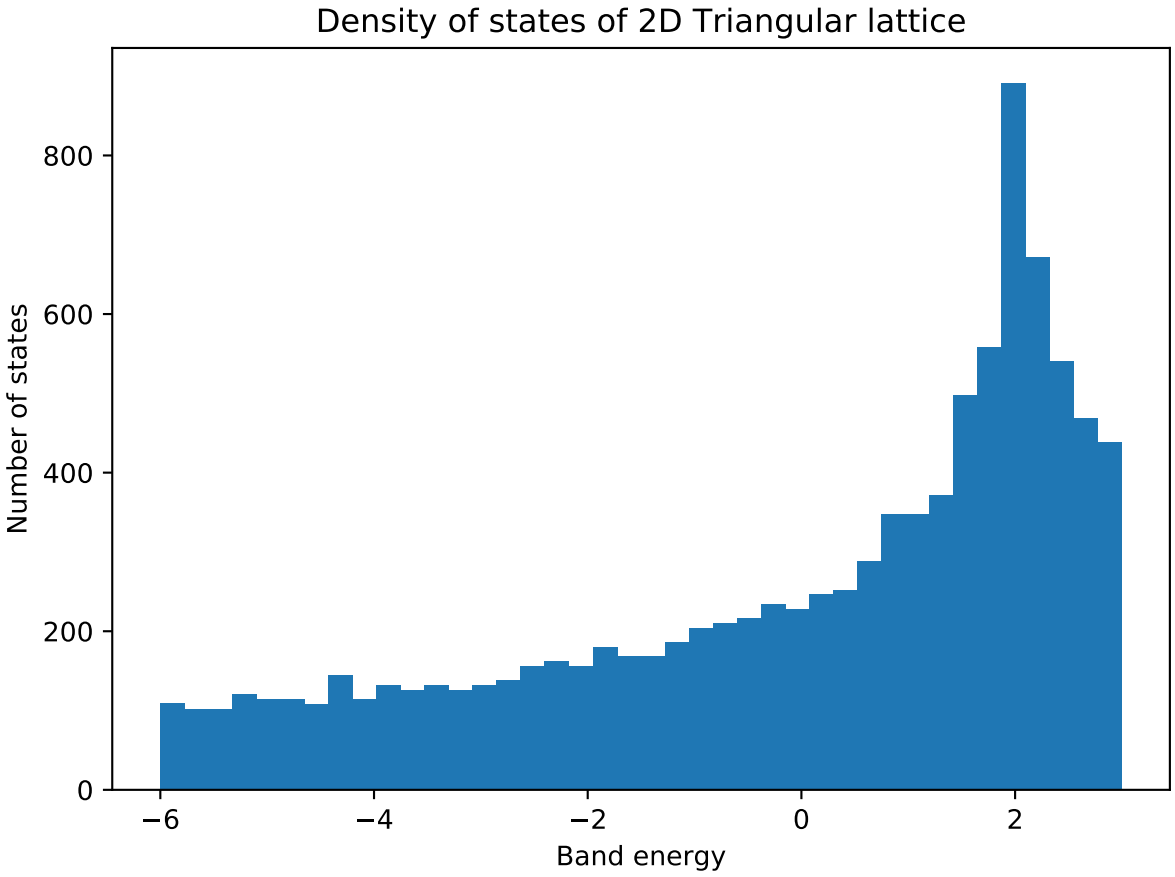

Figure 4: Density of states of the 2D triangular lattice.

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

Answer: A LEED pattern is essentially an image of the reciprocal space lattice (2 points). The reciprocal lattice, and therefore the LEED pattern, is already sketched in Figure 2 (2 points).