Utrecht University
Exam Solids & Solid Surfaces
January 28, 2014

Answer the questions in the spaces provided on the question sheets. If you run out of room for an answer, continue on the back of the page.

Name and student number: _____

Good luck!

Question 1: **Geometric structure** ..... *25 points*

(a) (3 points) Suppose you have done an STM experiment on an unknown material which has either a *bcc* or *fcc* crystal structure. The atomically resolved images show that each atom on the surface has 4 nearest neighbors in the surface plane, i.e. the surface has 4-fold rotational symmetry. Can you determine the crystal structure of the material based on this information alone? Explain.

***answer**: No (1 point). Both bcc and fcc crystals have planes where atoms have 4 nearest neighbors (2 points).*

(b) (2 points) Consider a one atomic layer thick Cu_2N sheet with the geometry as shown in Figure 1 below. This material can be grown on e.g. Cu(100). Indicate a unit cell in the figure.

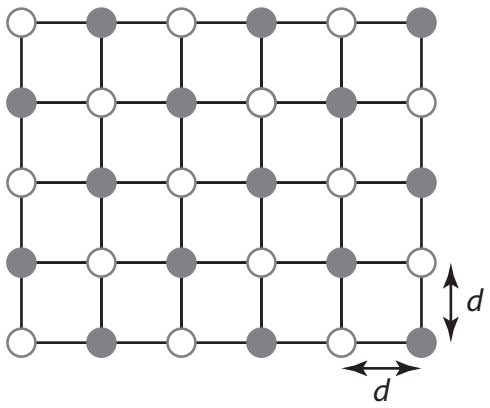

Figure 1: Geometry of a Cu_2N sheet. Cu and N atoms are indicated by filled and open circles, respectively.

(c) (4 points) Determine the unit cell vectors

***answer**:*

$$\begin{aligned} \mathbf{a}_1 &= (d, d) \\ \mathbf{a}_2 &= (d, -d) \end{aligned} \tag{1}$$

One point for each correct component.

(d) (11 points) Determine the lattice vectors of the reciprocal unit cell. Sketch the reciprocal unit cell and indicate the first Brillouin zone.

answer:

$$\mathbf{a}_i \cdot \mathbf{b}_j = 2\pi\delta_{i,j} \tag{2}$$

where i and j are indices that are either 1 or 2. This is a set of 4 equations. 1 point for each correct equation. This gives the following reciprocal unit cell vectors:

$$\begin{aligned} \mathbf{b}_1 &= \left(\tfrac{\pi}{d}, \tfrac{\pi}{d}\right) \\ \mathbf{b}_2 &= \left(\tfrac{\pi}{d}, \tfrac{-\pi}{d}\right) \end{aligned} \tag{3}$$

(4 points, one for each component of the two reciprocal unit cell vectors). The vectors $\boldsymbol{b}_1$ and $\boldsymbol{b}_2$ span a square grid (1 point). The first BZ corresponds to the Wigner-Seitz cell in reciprocal space (2 points).

(e) (5 points) K atoms can adsorb ontop of the Cu atoms of the Cu_2N sheet. In doing so, they donate an electron to the surface. Does this affect the work function? If so, why and how?

answer: Yes (1 point). The positively charged K atoms lower the dipole moment of the surface (4 points).

Question 2: **Graphene** ..... *26 points*

(a) (2 points) The unique electronic properties of graphene are related to the linear dispersion relation close to the Fermi level. What is the essential feature of graphene that leads to this linear dispersion?

***answer**: The honeycomb geometry.*

(b) (3 points) People refer to the electrons in graphene with energies close to the Fermi energy as *massless Dirac fermions*. Explain this term.

***answer**: The electrons, which are fermions (1 point) have a linear dispersion, as do photons. Photons have an effective mass of zero. By analogy, electrons in graphene with energies close to the Fermi energy have an effective mass of zero (1 point). Consequently, they should be described by relativistic quantum mechanics, i.e. by the Dirac equation (1 point).*

(c) (10 points) As shown in the exercise class, the dispersion relation of graphene close to the Fermi level is given by:

$$E(\mathbf{k}) = \hbar v_F \, |\mathbf{k}| \tag{4}$$

where v_F is the Fermi velocity ($\approx 10^6$ m s^{-1}) and $\mathbf{k}$ is the wave vector w.r.t. the K-point of the Brillouin zone. Based on the above, derive an expression for the density of states, $\rho(E)$, per unit cell of graphene. The area that each state occupies in $\mathbf{k}$-space, per unit area of the crystal, is equal to $\frac{4\pi^2}{3\sqrt{3}a^2} = \frac{2\pi^2}{A_c}$, where A_c is the area of the unit cell of graphene.

***answer**: The total number of occupied states N, is, in terms of the Fermi wave vector $\boldsymbol{k}_F$, given by:*

$$N = 2\pi \mathbf{k}_F^2 \tag{5}$$

where the factor 2 accounts for the spin degree of freedom (2 points). Divide this by the area per k-point per unit area of the crystal and take the derivative to obtain an expression for the density of states per unit wave vector:

$$\frac{\partial N}{\partial k} = \frac{2A_c}{\pi}\mathbf{k}_F \tag{6}$$

2 points. Realize that to obtain an expression for the density of states per unit energy, one needs an expression for $\frac{\partial k}{\partial E}$. This can be obtained from the the linear relation between the wave vector and energy:

$$\frac{\partial k}{\partial E} = \frac{1}{\hbar v_F} \tag{7}$$

2 points.

Hence, one obtains for the density of states:

$$\frac{\partial N}{\partial E} = \frac{\partial N}{\partial k}\frac{\partial k}{\partial E} = \frac{2A_c}{\pi}\frac{1}{\hbar v_F}k_F \tag{8}$$

2 points. Use again the linear relation between the wave vector and the energy to arrive at:

$$\frac{\partial N}{\partial E} = \frac{2A_c}{\pi}\frac{1}{\hbar^2 v_F^2}E \tag{9}$$

2 points.

(d) (4 points) Comment on the energy dependence of $\rho(E)$ of graphene. How does it relate to the energy dependence of a 2D free-electron gas?

***answer**: For graphene, the DOS close to the Fermi level is linearly dependent on energy (1 point). The DOS of a 2DEG increases in steps (1 point). In between the steps, the DOS is independent of energy (2 points).*

(e) (4 points) Figure 2 below shows a differential conductance spectrum of graphene. Is this spectrum consistent with the theoretically predicted energy dependence of $\rho(E)$? Explain.

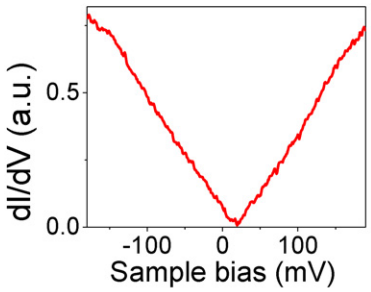

Figure 2: Differential conductantance spectrum of graphene as measured with scanning tunneling microscopy.

***answer**: Yes (1 point). $\frac{dI(V)}{dV} \propto \rho(E)$ (3 points).*

(f) (3 points) Consider Figure 2. What can you tell about the position of the Fermi level in this particular graphene sample? Relate this to the theoretically predicted position of the Fermi level.

***answer**: The minimum in the DOS corresponds to the location of the Dirac cone, which for this particular sample is located at positive bias (1 point). The Fermi level is located at zero bias (1 point). Hence, the material has lost some of its electrons (1 point).*

Question 3: **Free Electron Model** ..... *31 points*

(a) (3 points) Two potential wells are brought close together. The distance between them is L. The potential energy landscape is sketched in Figure 3 below. If the distance between the wells is small enough, there is a non-zero probability for electron tunneling, i.e. for the electron to move from the left well to the right well or vice versa.

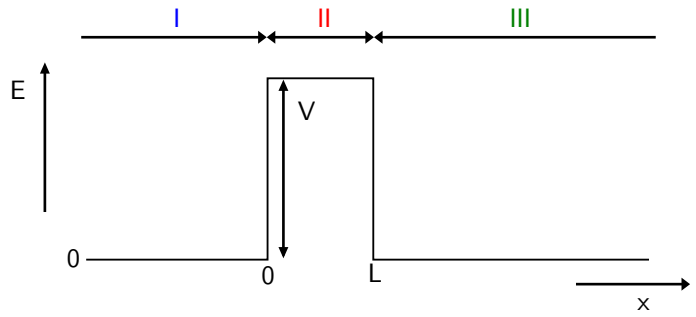

Figure 3: Electron tunneling between two potential wells.

The wave functions in the three regions are given by:

$$\begin{aligned} \psi_I(x) &= Ae^{ik_1x} + A'e^{-ik_1x} \\ \psi_{II}(x) &= Be^{k_2x} + B'e^{-k_2x} \\ \psi_{III}(x) &= Ce^{ik_3x} + C'e^{-ik_3x} \end{aligned} \tag{10}$$

Is there a relation between the wave vectors in region I and III? If so, which one and why?

***answer**: Yes (1 point). Energy conservation (1 point) demands that $k_1 = k_3$ (1 point).*

(b) (3 points) Give expressions for all wave vectors.

***answer**:*

$$\begin{aligned} k_1^2 &= \tfrac{2m}{\hbar^2}E \\ k_2^2 &= \tfrac{2m}{\hbar^2}(V-E) \\ k_3^2 &= \tfrac{2m}{\hbar^2}E \end{aligned} \tag{11}$$

1 point for each correct equation.

(c) (8 points) To get a measure for the tunneling probability, we will consider the probability current which is defined as:

$$j_x = \frac{1}{2m}\left[\psi^* \hat{p} \psi - \psi \hat{p} \psi^*\right] \tag{12}$$

with $\hat{p} = -i\hbar(\partial/\partial x)$ the momentum operator. Give expressions for the probability current in regions I and III:

***answer**: Insert the wave functions for regions I and III given under (a) into the equation to find:*

$$\begin{aligned} j_I(x) = \frac{i\hbar}{2m}\big[&\left(Ae^{-ik_1x} + A'e^{ik_1x}\right)\left(ik_1Ae^{ik_1x} - ik_1A'e^{-ik_1x}\right) - \\ &\left(Ae^{ik_1x} + A'e^{-ik_1x}\right)\left(-ik_1Ae^{-ik_1x} + ik_1A'e^{ik_1x}\right) \end{aligned} \tag{13}$$

2 points. This equation simplifies to:

$$\jmath_I(x) = \frac{\hbar k_1}{m}\left(A^2 - A'^2\right) \tag{14}$$

2 points. By analogy, one finds for region III:

$$\jmath_{III}(x) = \frac{\hbar k_1}{m}\left(C^2 - C'^2\right) \tag{15}$$

4 points.

(d) (6 points) The transmission coefficient, T, is simply the ratio between the probability for travelling in the positive x-direction (A^2, C^2) and travelling in the negative x-direction (A'^2, C'^2):

$$T = \frac{|C|^2}{|A|^2} = \frac{|C'|^2}{|A'|^2} \tag{16}$$

This represents the probability of an electron tunneling from left to right or from right to left.

How can you obtain an expression for the transmission coefficient, starting from the wave functions as given under (a)? Give the 4 starting equations.

***answer**: Make use of the fact that the wave function must be continous at both interfaces (2 points):*

$$\begin{aligned} A + A' &= B + B' \\ ik_1A - ik_1A' &= k_2B - k_2B' \\ Be^{k_2L} + B'e^{-k_2L} &= Ce^{ik_1L} + C'e^{-ik_1L} \\ k_2Be^{k_2L} - k_2B'e^{-k2L} &= ik_1Ce^{ik_1L} - ik_1C'e^{-ik_1L} \end{aligned} \tag{17}$$

1 point for each correct equation.

(e) (6 points) One finally obtains the following expression for T:

$$T = \frac{1}{1 + \frac{\left(k_1^2+k_2^2\right)^2}{\left(4k_1^2k_2^2\right)} \sinh^2\left(k_2 L\right)} \tag{18}$$

Show that for a barrier that is either very long or very high, that the transmission coefficient can be approximated by:

$$T \approx \frac{16E\left(V-E\right)}{V^2} e^{-2k_2 L} \tag{19}$$

You may find the definition of $\sinh(x)$ useful:

$$\sinh(x) = \frac{e^x - e^{-x}}{2} \tag{20}$$

***answer**: Insert the definition of* $\sinh(x)$ *to find:*

$$T = \frac{1}{1 + \frac{\left(k_1^2+k_2^2\right)^2}{\left(4k_1^2k_2^2\right)} \frac{\left(e^{k_2 L} - e^{-k_2 L}\right)^2}{4}} \tag{21}$$

1 point. For a very long or very high barrier: $k_2 L >> 1$ *(1 point). Hence, the* $e^{-k_2 L}$ *term can be neglected. The above expression simplifies to:*

$$T \approx \frac{16k_1^2k_2^2}{\left(k_1^2+k_2^2\right)^2} e^{-2k_2 L} \tag{22}$$

2 points. Insert the expression for the wave vectors to arrive at:

$$T \approx \frac{16E\left(V-E\right)}{V^2} e^{-2k_2 L} \tag{23}$$

2 points.

(f) (5 points) The situation as depicted in Figure 3 resembles the scanning tunneling microscope. The tunneling current that flows is directly proportional to the transmission coefficient. Based on Figure 3 and equation 19, how can STM be used to measure the workfunction of a material?

***answer**: Realize that the depth of the potential well, V, corresponds to the work function (1 point). The absolute distance between tip and sample is unknown in STM (1 point). Hence, it's not possible to directly relate the current at a given point to the work function. Instead, one measures the current as a function of tip-sample distance (2 points). k_2 and hence the work function can be obtained by determining the slope of a plot of* $\ln I$ *versus distance (1 point).*