Project 2. Electrostatic Energy in Ionic Crystals

Notes on project:

1. This is a group project. Each group may consist of either two or three students. Each group shall submit a single report in pdf format.
2. Experimental measurements may be done in our laboratories or using other resources as in the case of the first project.
3. Deadline of the report submission: May 21, 2023, 23:59.

General Task: Studying the electrostatic energy in multi-particle systems (crystals).

Part 1. NaCl Salt Crystal. Let's consider the electrostatic energy of an ionic lattice. An ionic crystal like NaCl consists of positive and negative ions which can be thought of as rigid spheres. They attract electrically until they begin to touch; then there is a repulsive force that goes up very rapidly if we try to push them closer together.

For our simplified model, we imagine a set of rigid spheres that represent the atoms in a NaCl salt crystal, see **Figure 1**.

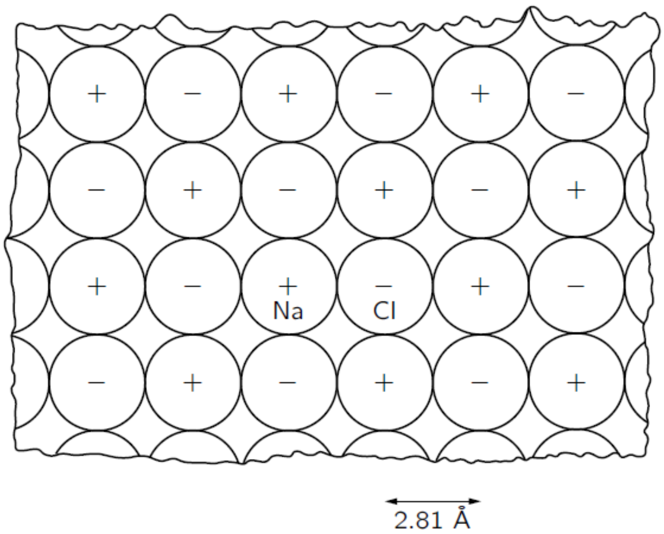

Figure 1. Cross section of a salt crystal on an atomic scale. The checkerboard arrangement of Na and Cl ions is the same in the two cross sections perpendicular to the one shown.

Task 1. The Madelung Constant for 1D Crystal. Consider 1D lattice for the NaCl crystal, see **Figure 2**. Here the spacing parameter $R_e = 2.81 \times 10^{-8}$ cm.

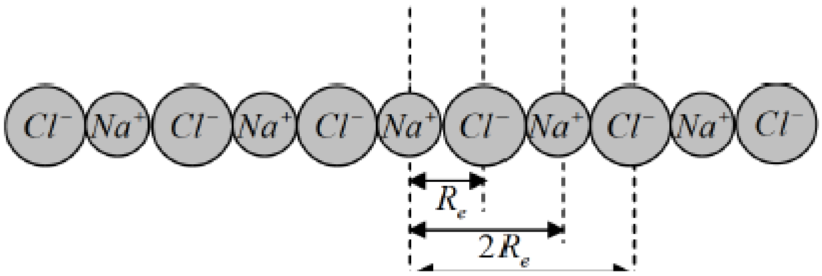

Figure 2. 1D lattice for NaCl crystal.

Let us take one sodium ion as a reference body and develop the equation of its ***electrostatic potential energy*** *U* in the infinite linear chain of ions. In this case we can write for this ion the energy of electrostatic interaction of atoms in the crystal in the form:

$$U = -\alpha \frac{q^2}{4\pi\varepsilon_0 R_e} \quad . \tag{1}$$

The electrical charges q of the ions are equal to the electron charge e.

Derive the analytical series for the electrostatic potential energy (1) for all pairs of ions in the infinite 1D chain, make the summation of the infinite series, and find the constant α explicitly (it's called the ***Madelung constant***) for the infinite 1D crystal.

Task 2. The Madelung Constant for 2D Crystal. Make the numerical evaluation of the Madelung constant α in Equation (1) for 2D infinite NaCl crystal, see **Figure 3**.

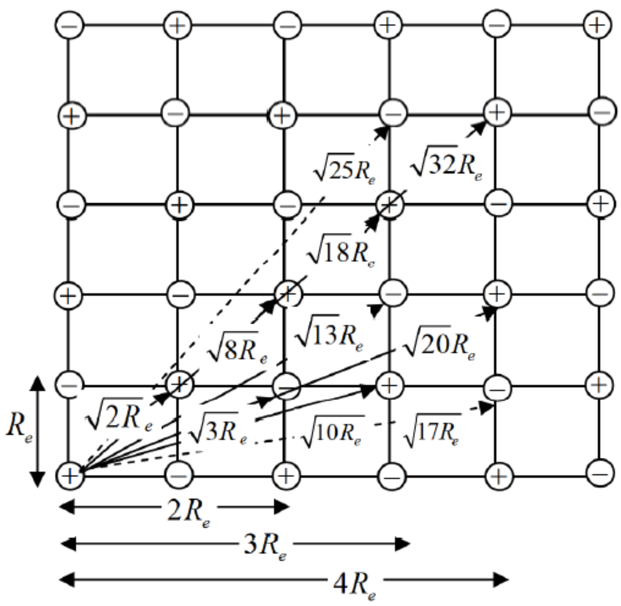

Figure 3. 2D lattice for NaCl crystal.

Task 3a. Equivalent resistance of infinitely large resistor networks. Let the electrons experience an effective resistance of r_0 while traveling from a Na atom to a Cl atom or vice versa in a 2D lattice as shown in Figure 3. Using a simulation tool, form a network of resistors having

4, 16, 64, 128, and 256 nodes (each node corresponding to an atom in the lattice) and calculate the equivalent resistance. Present your simulation structure and results in your report. Interpret your results to explain how the equivalent resistance varies as the number of nodes increases.

Task 3b. Equivalent resistance measurement of large resistor networks. Form a resistive network composed of 4 and 16 nodes made of resistors of your choice. Develop a test method to measure the equivalent resistance and verify your predictions in part 3a in the laboratory environment. Explain the test methodology for the measurement and show your proof of measurements in your report.

Task 4a. Equivalent capacitance of infinitely large capacitor networks. Let an effective capacitance of C_0 be present between a Na atom and a Cl atom in a 2D lattice as shown in Figure 3. Using a simulation tool, form a network of capacitors having 4, 16, 64, 128, and 256 nodes (each node corresponding to an atom in the lattice) and calculate the equivalent capacitance. Present your simulation structure and results in your report. Interpret your results to explain how the equivalent capacitance varies as the number of nodes increases.

Task 4b. Equivalent capacitance measurement of large capacitor networks. Form a capacitive network composed of 4 and 16 nodes made of capacitors of your choice. Develop a test method to measure the equivalent capacitance and verify your predictions in part 4a in the laboratory environment. Explain the test methodology for the measurement and show your proof of measurements in your report.

Part 2. Studying Van der Waals (molecular) bonding for the inert gas crystal. Now let's consider a crystal of inert gases, which are characterized by *van der Waals* (*or molecular*) bonding: the noble gases such as neon (Ne), argon (Ar), krypton (Kr), and xenon (Xe) are good examples of such crystals.

What holds atoms in an inert gas crystal together? A pair of inert gas atoms (1 and 2) separated by distance r can be represented with the model of the coupling between the two dipoles, one caused by a fluctuation, and the other induced by the electric field produced by the first one, resulting in the attractive force, which is called the ***van der Waals force***. It is given by the potential:

$$U(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] \quad . \tag{2}$$

Eq.(2) is called the **Lennard-Jones potential**. Here σ and ε are positive constants, which are supposed to be known.

Task 5.

(a) Using Equation (2), derive the analytical equation for the force F for the electrostatic potential energy (2) as a function of the distance r (if the mass of the atom is m and the electrical charge is e).

(b) For the functions $U(r)$ and $F(r)$ investigate the extrema (minima and maxima) properties, and plot both functions.

(c) Find the equilibrium distant r_{eq} for the Lennard-Jones potential.

(d) Write the equation for the force **F** components F_x, F_y, F_z in the Cartesian coordinates (considering the spherical symmetry of this force with respect to its radial measure r).

(e) Find the Cartesian components of the gradient vector for $U(r)$.

(f) Find the work W which is done by the Lennard-Jones force to transfer the electrical charge e from the initial position $r = \sigma$ to infinity.

Part 3. Toy Model for the Resistance in the Cristal Lattice. In Figure 4 you can see the simple ‘toy’ model, which reflects in a peculiar way the process of interaction of electrons in a metal with oscillating ions of the crystal lattice.

In this model, there is some particle (the white ball in Figure 4 representing an electron), which moves uniformly in a straight line and uniformly through some conditional “corridor” (the direction of its movement is indicated by the arrow). In the “corridor”, there are ions of the lattice (the black balls) that perform oscillatory (reciprocating) movements, as lined with arrows.

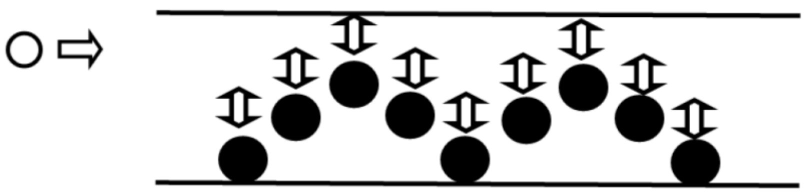

Figure 4. Toy model for the resistance in the crystal lattice.

Let’s show how this model uniquely reflects the resistance of the tall to the movement of electrons under the action of an external electric field (or resistance to the flow of electric current through a metal). As is known, the electrical resistance for the moving electrons is caused by thermal vibrations of ions in the crystal lattice. Therefore, the white ball is schematically reflecting the motion of an electron under the action of an electric field, and the black balls represent the oscillating metal ions (due to the thermal vibrations).

Task 4. Let’s assume that with decreasing temperature, the magnitude of the black ball oscillations decreases. Develop arguments that with such a decreasing temperature change, the electrical resistance of the metal decreases, as it is shown in Figure 5. Why we can suppose a simple linear plot?

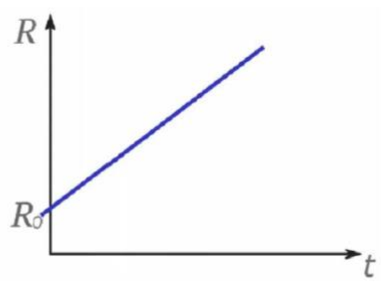

Figure 5. Dependence of the resistance R (Ohm) vs temperature t (Celsius) in the metals.