

Worksheet
Practical I

VESTA is a tool for visualization and analysis of crystal structures.

You are given the structure files for two materials, one Aluminum (Al) and sodium chloride (NaCl).

Open them one-by-one in VESTA, and obtain the following information. While answering each question, write in your own words, how you obtained this information in the VESTA tool.

1. What are the lattice parameters of Al and NaCl.
2. Obtain the inter-atomic distances (Al-Al and Na-Cl, Na-Na and Cl-Cl) in the two structures.
3. Obtain the values of Al-Al-Al, Na-Cl-Na and Na-Na-Cl angles.
4. Visualize the Al structure along the c axis, and now rotate the structure about c-axis by 30° and b-axis by 20° . Save the final orientation in a .png file. Take a screenshot and paste it as the answer.
5. In the Al structure, consider the atom at the position (0.5,0.0,0.5). Write the coordinates of all its nearest neighbours. Explain the steps followed.
6. In the Al structure, construct displacement vectors on the atoms at (0.0,0.0,0.0) and (0.5, 0.0, 0.5) along the [1 1 0] and [1 1 1] directions respectively, each with scaling factor 0.35. Explain all the steps involved. Repeat the same for the NaCl structure.
7. In the Al structure, construct (2 0 0), (1 1 0) and (1 1 1) planes. Explain the steps involved. Repeat the same for the NaCl structure.