

HomeWork #.3

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1 HEXAGONAL LATTICE AND PRIMITIVE CELL.

1. For a simple hexagonal lattice we can choose the following primitive vectors: $\mathbf{a}_1 = \sqrt{3}/2a\mathbf{e}_x + 1/2a\mathbf{e}_y$, $\mathbf{a}_2 = -\sqrt{3}/2a\mathbf{e}_x + 1/2a\mathbf{e}_y$, $\mathbf{a}_3 = c\mathbf{e}_z$. What volume does the primitive unit cell have?
2. Deduce the primitive vectors for the reciprocal lattice. Describe it from a point of view of the W-Z. construction.
3. Sketch the 1st Brillouin zone.

2 CRYSTAL STRUCTURE OF BaTiO_3

Barium titanite BaTiO_3 crystalizes in such a structure that Ba atoms sit at the corners of a cube with Ti atoms at the cube center and O atoms in the centers of its faces.

1. Describe this structure with a suitable lattice and basis.
2. Determine the intensity relationship between the first four Bragg reflections with the of help of this structure factor. The following form factors apply to the atoms: $f_{\text{Ba}} = 7f_{\text{O}}$ and $f_{\text{Ti}} = 3f_{\text{O}}$.