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Structure and Properties of Functional Materials

Exercise Set 1

Friday, 11 January, 2013

1. *For discussion:*
   (a) Suppose two diffraction patterns of the same crystal are measured: one recording all spots with $Q \leq 7\,\text{Å}^{-1}$, the other recording all spots with $Q \leq 10\,\text{Å}^{-1}$. Explain why the uncertainty in the calculated atomic positions will be greater for the first than for the second experiment.
   (b) How would you expect the diffraction patterns of a block-shaped crystal (like a grain of salt) and a long, needle-shaped crystal of the same material to differ?

2. Uranium tetrafluoride, which in its molten state can be used to fuel molten-salt nuclear reactors, has room-temperature lattice vectors (in Å)

$$\begin{aligned}\mathbf{a} &= 12.81\mathbf{i}\\ \mathbf{b} &= 8.40\mathbf{j}\\ \mathbf{c} &= -6.34\mathbf{i} + 8.67\mathbf{k}\end{aligned}$$

   where $\mathbf{i}, \mathbf{j}, \mathbf{k}$ are the orthogonal unit vectors. Calculate the reciprocal lattice vectors for this crystal. Sketch them and the real lattice vectors on the same diagram. Calculate the real and reciprocal cell volumes.

3. What is the maximum value of Q measurable with copper $K\alpha$ radiation of wavelength $\lambda = 1.5418\,\text{Å}$? Estimate how many distinct diffraction spots would theoretically be measurable if a crystal of uranium tetrafluoride (see the previous question) were put in a beam of this radiation.

4. Let

$$f(x) = \begin{cases} e^{-x} & x \geq 0 \\ 0 & \text{otherwise;} \end{cases} \qquad g(x) = \begin{cases} xe^{-x} & x \geq 0 \\ 0 & \text{otherwise.} \end{cases}$$

   (a) Find the Fourier transform of $f(x)$.
   (b) Show that $(f \otimes f)(x) = g(x)$.
   (c) Hence use the convolution theorem to evaluate the Fourier transform of $g(x)$. Check your answer by direct calculation.