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SCHOOL OF PHYSICS AND ASTRONOMY

Structure and Properties of Functional Materials

Homework Set 1

Due Wednesday, 16 January, 2013 by 4 p.m.

Problem 1: Terms and definitions (8 marks)

Explain the following terms or concepts, giving an example of their significance in condensed matter physics:

(a) Lattice (4)

(b) Convolution theorem (4)

Problem 2: Symmetry in real and reciprocal space (15 marks)

(a) Suppose that $f(x)$ is a *centrosymmetric* function; that is, that for all x, $f(x) = f(-x)$. Let $F(Q)$ be its Fourier transform. How are $F(Q)$ and $F(-Q)$ related? (5)

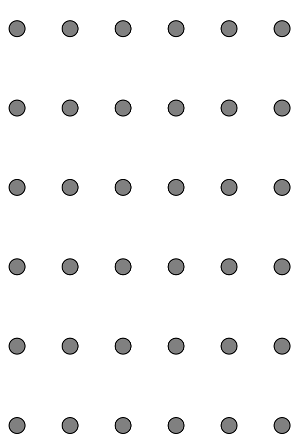
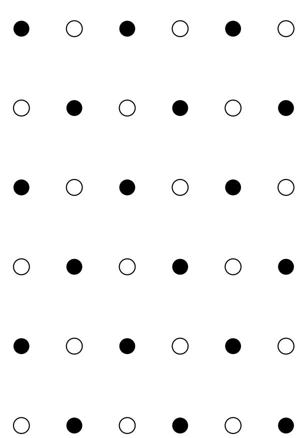
(b) Now suppose that, as well as being centrosymmetric, f is also real. Using results from lectures and from the previous part, what can we say about F now? (3)

(c) Let $f(x) = \exp(-|x|)$. Calculate $F(Q)$, the Fourier transform of f. Does it behave as we expect, given that f is real and centrosymmetric? Is $F(0)$ what we expect? (7)

Problem 3: Real and reciprocal lattices (10 marks)

For each of the following pairs of "crystal structures" in one and two dimensions, sketch the real lattices (on the same diagram) and reciprocal lattices (on the same diagram, different from the first one). On your diagrams, indicate the real and reciprocal lattice vectors.

(a)  and  (4)

(b)  and  (6)

Problem 4: Magnesium oxide nanoparticles (7 marks)

The diagram below is taken from a 1946 paper in the *Journal of Applied Physics* by Birks and Friedman. It shows X-ray diffraction peaks from two samples of magnesium oxide nanoparticles prepared at different temperatures.

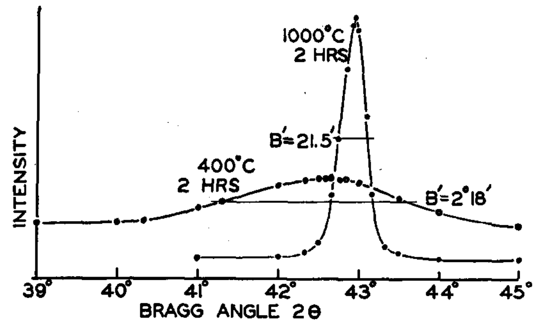


FIG. 9. Typical diffraction lines from magnesium oxide converted from the carbonate at 400°C and 1000°C. The intensity was measured with a Geiger counter at the points shown on the curves.

(a) Magnesium oxide has a cubic lattice with $a = b = c = 4.212\,\text{Å}$. Calculate the reciprocal lattice parameter a^* and hence the value of Q for the (200) diffraction peak. (2)

(b) Calculate the scattering angle 2θ at which this peak would be observed using Cu $K\alpha$ radiation ($\lambda = 1.5418\,\text{Å}$), and hence show that this is the diffraction peak shown in the figure. (2)

(c) Which of the two samples (the one generated at 400 °C or the one generated at 1000 °C) contained smaller nanoparticles? Explain your answer. (3)