STATE UNIVERSITY OF NEW YORK AT BUFFALO

Department of Mechanical and Aerospace Engineering

MEA 589 Diffraction, Microscopy and Spectroscopy Techniques

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HOMEWORK NO. 3

Problem 1 (30%)

Derive the expression for the distance between adjacent direct lattice planes perpendicular to the same reciprocal lattice vector of

(6%) (i) the cubic system,

(6%) (ii) the tetragonal system,

(6%) (iii) the orthorhombic system,

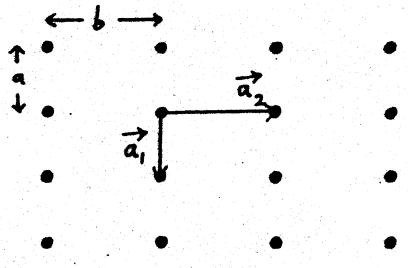
(12%) (iv) the hexagonal system

The derivation should not be by geometry. Rather, Eq. (2.36) in the notes should be used.

Hint: Start by writing the fundamental translation vectors in the direct lattice under consideration in the (x,y,z) coordinate system. Obtain the corresponding fundamental translation vectors in reciprocal space. Your answer should be in terms of m_1, m_2, m_3 and the lattice parameters in direct space.

Problem 2 (30%)

Given a two-dimensional lattice with lattice parameters a and b along the $\vec{a}_1$ and $\vec{a}_2$ directions, respectively.



(a) Sketch the lattice "planes" described by the Miller Indices (2,3), (1,2), (4,1).

(b) Write an expression for the reciprocal lattice vector perpendicular to the (2,3) "plane".

(c) What is the reciprocal lattice vector perpendicular to the (m_1,m_2) "plane"?

(d) Find the angle between the (2,3) "plane" and the (1,2) "plane".

(e) Find the angle between the (4,1) "plane" and the (1,2) "plane".

(f) What is the distance between adjacent (1,2) "planes"?

Problem 3 (40%)

SnO_2 is a material which is presently being investigated for use in solar energy conversion devices due to its transparency in the visible wavelengths and high reflectivity in the infrared. Look up the structure of SnO_2 in Wyckoff, Crystal Structures, Vol. I (available in the Engineering and Science Library). QD921.W82 1963

(a) Give the fundamental translation vectors for the smallest unit cell and express the positions of the 6 atoms per unit cell.

(b) Find the corresponding unit cell in reciprocal space.

(c) Consider the expansion of a function which is periodic in the SnO_2 structure (e.g. the periodic potential).

Treat the potential to be of the form:

$$f(r) = \sum_{j}^{\text{all atoms in crystal}} C_j \delta(\vec{r} - \vec{r}_j),$$

where $\vec{r}_j$ is defined as the position of the j^{th} atom within the crystal, $C_j = A$, for all $\vec{r}_j$ corresponding to the location of the Sn atoms, and $C_j = B$ for the $\vec{r}_j$ corresponding to the location of O atoms. Which, if

any, of the Fourier coefficients, $F_{\vec{G}_m}$, vanish for $\vec{G}_m = (1,1,1)$, $\vec{G}_m = (1,0,2)$, $\vec{G}_m = (1,1,0)$?

Explain the physical significance of the vanishing of a Fourier component.

Note: $\int \delta(\vec{r} - \vec{r}_j)\vec{dr} = 1$ if $\vec{r} = \vec{r}_j$

$= 0$ otherwise.