PHYS 321 Interplanar spacing & H-like Spectra Name:\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

1. For the cubic system, derive expressions for the interplanar spacings for (100), (200), (110), and (111) planes and show that they agree with what is given by the following equation: $d\_{hkl}=\frac{a}{\sqrt{h^{2}+k^{2}+l^{2}}}$



2. Derive the following expression for the wavelength of Hydrogen like spectra.
$$\frac{1}{λ}=RZ^{2}\left(\frac{1}{n\_{f}^{2}}-\frac{1}{n\_{i}^{2}}\right)$$

PHYS 321 X-ray Diffraction Name:\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

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| Braggs’s Law | Inter-planar Spacing | Hydrogen Like Spectra (R= 1.097 x 107 m-1) |
| $$2d\_{hkl}Sinθ=nλ$$ | $$d\_{hkl}=\frac{a}{\sqrt{h^{2}+k^{2}+l^{2}}}$$ | $$\frac{1}{λ}=RZ^{2}\left(\frac{1}{n\_{f}^{2}}-\frac{1}{n\_{i}^{2}}\right)$$ |

3. The 2ϴ values in degrees for first order diffraction peaks are given below for a metal with cubic structure, using X-rays from Cu-Kα radiation (Z = 29): 44.48, 51.83, 76.35, 92.9, 98.4, 121.87, 144.54, 155.51.

(a) Determine the wavelength of the X-rays used.

(b) Derive an expression for $\frac{Sin^{2}θ}{h^{2}+k^{2}+l^{2}}$ .
(c) Complete the table below.

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| 2θ (deg.) | θ (rad) | Sin2θ | Normalize | ClearFractions | h2+k2+l2 | (hkl) | $$\frac{Sin^{2}θ}{h^{2}+k^{2}+l^{2}}$$ |
| 44.48 |  |  |  |  |  |  |  |
| 51.83 |  |  |  |  |  |  |  |
| 76.35 |  |  |  |  |  |  |  |
| 92.9 |  |  |  |  |  |  |  |
| 98.4 |  |  |  |  |  |  |  |
| 121.87 |  |  |  |  |  |  |  |
| 144.54 |  |  |  |  |  |  |  |
| 155.51 |  |  |  |  |  |  |  |

(d)Determine the crystal structure.

(e)Determine the lattice constant.
(f) Determine the ionic radius.
(g) Identify the metal.

PHYS 321 X-ray Diffraction Name:\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

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| Braggs’s Law | Inter-planar Spacing | Hydrogen Like Spectra (R= 1.097 x 107 m-1) |
| $$2d\_{hkl}Sinθ=nλ$$ | $$d\_{hkl}=\frac{a}{\sqrt{h^{2}+k^{2}+l^{2}}}$$ | $$\frac{1}{λ}=RZ^{2}\left(\frac{1}{n\_{f}^{2}}-\frac{1}{n\_{i}^{2}}\right)$$ |

4. The 2ϴ values in degrees for first order diffraction peaks are given below for a metal with cubic structure, using X-rays from Ag-Kα and (Z = 47):

(a) Determine the wavelength of the Kα and Lα X-rays (need this for (g)).(b) Derive an expression for $\frac{Sin^{2}θ}{h^{2}+k^{2}+l^{2}}$ .

(c)Determine the crystal structure.

(d)Determine the lattice constant.
(e) Determine the ionic radius.
(f) Identify the metal.
(g) At what angle be the first reflection if, instead of Kα radiation, Lα radiation is used?

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| 2θ (deg.) | θ (rad) | Sin2θ | Normalize | ClearFractions | h2+k2+l2 | (hkl) | $$\frac{Sin^{2}θ}{h^{2}+k^{2}+l^{2}}$$ |
| 14.10 |  |  |  |  |  |  |  |
| 19.98 |  |  |  |  |  |  |  |
| 24.54 |  |  |  |  |  |  |  |
| 28.41 |  |  |  |  |  |  |  |
| 31.85 |  |  |  |  |  |  |  |
| 34.98 |  |  |  |  |  |  |  |
| 37.89 |  |  |  |  |  |  |  |
| 40.61 |  |  |  |  |  |  |  |



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| Braggs’s Law | Inter-planar Spacing |
| $$2d\_{hkl}Sinθ=nλ$$ | $$d\_{hkl}=\frac{a}{\sqrt{h^{2}+k^{2}+l^{2}}}$$ |

5. The 2ϴ values in degrees for first order diffraction peaks are given above for [SrTiO3](https://lippmaa.issp.u-tokyo.ac.jp/sto/), with cubic structure, using X-rays of wavelength 0.154 nm.

(a) Derive an expression for $\frac{Sin^{2}θ}{h^{2}+k^{2}+l^{2}}$

(b) Determine the crystal structure. (c)Determine the lattice constant.

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| --- | --- | --- | --- | --- | --- | --- | --- |
| 2θ (deg.) | θ (rad) | Sin2θ | Normalize | ClearFractions | h2+k2+l2 | (hkl) | $$\frac{Sin^{2}θ}{h^{2}+k^{2}+l^{2}}$$ |
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