Indexing an XRD pattern:

Indexing is the process of determining the unit cell dimensions from the peak positions. In order to do this you must first assign the hkl Miller indices.

1. Find your peaks, list the 2θ values

2. Find θ

3. Calculate the d-spacing for each peak using Bragg’s Law

4. Find 1000/d2

5. Find a common factor that (1000/d2) may be divided by for each peak that gives a whole number. (A bit of guess-and-check)

6. Using the whole numbers once divided by a common factor (CF), find combinations of hkl that satisfy: whole number = h2 + k2 + l2 (a bit of guess-and-check)

7. Look at hkl’s and see if these correspond to any systematic absences due to centering. (see attached)

8. Determine the cell length, a. (formula attached)

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| 2θ | θ | d | 1000/d2 | (1000/d2)/CF | hkl |
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From the lab:

Bragg’s Law (Equation 4.1) tells us the location of a peak with indices hkl, θhkl, is related to the d-spacing:

λ = 2 dhkl sin θhkl  (1.1)

The d-spacing is also related to hkl indices by Equation 4.2:

 $\frac{1}{d^{2}}=\frac{h^{2 }+ k^{2 }+l^{2 }}{a^{2 }}$ (1.2)

By combining and rearranging these equations we may get

$\frac{sin^{2}θ}{h^{2 }+ k^{2 }+l^{2 }}=\frac{λ^{2}}{4a^{2}}$ (1.3)

Using educated guessing we need to find values of h, k, and l that give a constant when each is divided by sin2θ. We may then use this to solve for the lattice parameter, a.

Systematic absences – Centering

If the lattice is not primitive certain classes of hkl peaks will be missing.

|  |  |
| --- | --- |
| Centering | Allowed Peaks |
| I centered | Peaks where h+k+l is an even number |
| F centered | Peaks where hkl are either all even #s or all odd #s |
| C centered | Peaks where h+k is an even number |
| B centered | Peaks where h+l is an even number |
| A centered | Peaks where k+l is an even number |
| R centered | Peaks where –h+k+l is a multiple of 3 |