- 短信 (Communication)

強度資料의 數 計算

徐日煥, 李珍昊, 秋錦洪, 李正秀, 成百石, 林星秀, 柳保盈, 朴晶蘭
金文執*, 趙素羅*

忠南大學校 自然科學大學 物理學科, 大田 305-764

*順天鄕大學校 自然科學大學 物理學科, 溫陽 336-600

Calculation of the Number of Intensity Data

Il-Hwan Suh, Jin-Ho Lee, Geum-Hong Choo, Jeong-Su Lee,
Baek-Seok Seong, Sung-Su Lim, Bo-Young Ryu, Jeong-Ran Park,
Moon-Jib Kim* and So-Ra Cho*

Department of Physics, Chungnam National University Daejeon 305-764 Korea

**Department of Pysics, Soonchunhyang University Onyang 336-600 Korea*

秒 錄

結晶構造解析을 하는데 必要하여 測定하여야할 回析强度의 數를 미리 알수있으면 自動 4軸回析分析計를 使用하여 X-線 回析强度를 募集하기 爲한 條件을 選擇하는데 매우 도움이 된다.

이 論文은 非對稱單位內의 募集可能한 强度資料의 數를 計算하는 方法을 提示하였다.

Abstract

The knowledge on the total number of necessary and collectable reflections for the crystal structure analysis is greatly helpful in choosing the conditions for X-ray intensity data collection using automatic four circle diffractometer.

In this paper, we represent a method to calculate the total number of collectable intensity data in an asymmetric unit.

Ⅰ. Introduction

Since a reciprocal lattice point corresponds to a reflection plane in a real space, the total number of reflections within the limiting sphere can be calculated by dividing the volume of the limiting sphere by the reciprocal lattice volume of a sample. The number of reflections, however, is reduced by taking only an asymmetric unit of intensity data and by eliminating the systematically absent reflections due to the symmetry of the Bravais lattice, and furthermore, by limiting the range of Bragg angle.

The methods shown previously are incomplete and even contain error[1, 2]. This paper reports a method to calculate the total number of collectable reflections in an asymmetric unit with the limit of Bragg angle and the reflection conditions for Bravais lattices.

Ⅱ. Theory

The volume of a reciprocal lattice space of a crystal limited by Bragg angle θ is $Vr^* = (4\pi/3)\, r^{*3}$ as shown in Fig. 1, where $r^* = (2 \sin \theta)/\lambda$ and λ is the wavelength of X-ray.

If V and V* are the volumes of a real and a reciprocal lattice unit cells of a sample, respectively, the total number N of reciprocal lattice points in the sphere Vr* is obtained by multiplying the volume Vr* by V since $V \cdot V^* = 1$.

The intensity patterns of 230 space groups are classified into 14 different kinds of point groups with an inversion center and, because of their symmetries, the asymmetric unit of intensity data of each point group represents only a certain fraction of the total number of reciprocal lattice points as shown in Table 1[3].

Table 1. The fraction f of reciprocal lattice space belonging to the asymmetric unit of Laue group.

Crystal system	Laue Group	f
Triclinic	$\bar{1}$	1/2
Monoclinic	2/m	1/4
Orthorhombic	mmm	1/8
Tetragonal	4/m	1/8
	4/mmm	1/16
Trigonal	$\bar{3}$ (R) $\bar{3}$ (H)	1/6
	$\bar{3}$m (R) $\bar{3}$1m (H) $\bar{3}$m1 (H)	1/12
Hexagonal	6/m	1/12
	6/mmm	1/24
Cubic	m$\bar{3}$	1/24
	m$\bar{3}$m	1/48

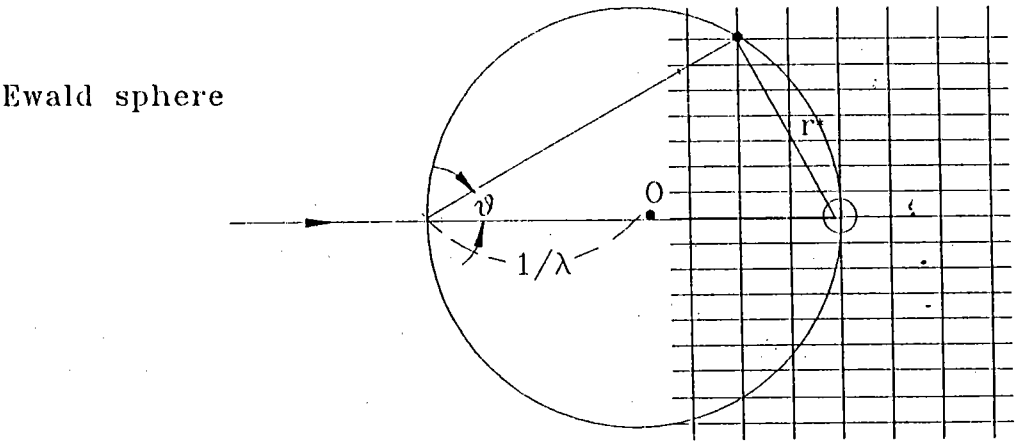

Fig 1. The reciprocal lattice points within the sphere with the radius $r^* = (2 \sin \theta)/\lambda$ are to be diffracted in a four-circle diffractometer.

If the Bravais lattice of a crystal is known, the number of reflections can be further reduced by applying the corresponding reflection conditions shown in Table 2.

Table 2. The reducing rate S of the number of reflections by Bravais lattice

Bravais lattice	reflection conditions	S
Primitive (P)	none	1
A-face centered (A)	$k+l$ = 2n	1/2
B-face centered (B)	$h+l$ = 2n	1/2
C-face centered (C)	$h+k$ = 2n	1/2
Body centered (I)	$h+k+l$ = 2n	1/2
All-face centered (F)	h, k, l: all even or all odd	1/4
triply primitive (TPR) rhombohedral	$h+k+l$ = 3n	1/3
hexagonal close (HCP) packed	$h-k$ = 3n, l = 2n or $h-k$ = 3n±1	5/6
obverse setting (OSH) hexagonal	$-h+k+l$ = 3n	1/3
reverse setting (RSH) hexagonal	$h-k+l$ = 3n	1/3
hexagonally (HC) centered	$h-k+l$ = 3n	1/3

Therefore, the total number N of the reciprocal lattice points to be taken for the crystal structure analysis is given as follows:

$$N = \frac{4\pi}{3}(r_2^{*3} - r_1^{*3}) \cdot V \cdot f \cdot S = (Vr_2^* - Vr_1^*) \cdot V \cdot f \cdot S,$$

where Vr_2^* and Vr_1^* are the reciprocal lattice volumes corresponding to the upper and lower limits of Bragg angles, respectively, and their values are given in Table 3.

Table 3. The volume of the reciprocal lattice sphere of crystal corresponding to Bragg angle.

θ (°)	0.71069 Å (Mok α)		1.5418 Å (Cuk α)	
	r*	V_r*	r*	V_r*
1	0.049114	0.000496	0.022639	0.000049
2	0.098213	0.003968	0.045271	0.000389
3	0.147282	0.013383	0.067889	0.001311
4	0.196306	0.031688	0.090487	0.003103
5	0.245271	0.061805	0.113057	0.006053
10	0.488675	0.488820	0.225254	0.047875
12	0.585098	0.839025	0.269700	0.082173
15	0.728360	1.618552	0.335736	0.158520
20	0.962502	3.735020	0.443663	0.365805
23	1.099583	5.568935	0.506851	0.545417
24	1.144625	6.281709	0.527613	0.615225
25	1.189318	7.046651	0.548214	0.690143
26	1.233649	7.864371	0.568649	0.770230
27	1.277605	8.735309	0.588910	0.855529
28	1.321171	9.659750	0.608992	0.946068
29	1.364335	10.637800	0.628888	1.041857
30	1.407083	11.669390	0.648593	1.142890
35	1.614140	17.616190	0.744035	1.725315
40	1.808911	24.793650	0.833815	2.428270
45	1.989916	33.006000	0.917248	3.232581
48	2.091333	38.314080	0.963996	3.752450
49	2.123878	40.130780	0.978998	3.930376
50	2.155777	41.966220	0.993701	4.110137
51	2.187018	43.817310	1.008102	4.291432
52	2.217593	45.680870	1.022196	4.473948
60	2.437140	60.635910	1.123395	5.938632
61	2.461325	62.459100	1.134544	6.117194
62	2.484761	64.260300	1.145347	6.293603
63	2.507441	66.035970	1.155800	6.467509
64	2.529356	67.782640	1.165902	6.638577
65	2.550501	69.496860	1.175649	6.806464
66	2.570869	71.175160	1.185038	6.970839
67	2.590454	72.814220	1.194065	7.131367
68	2.609250	74.410720	1.202729	7.287727
69	2.627251	75.961430	1.211027	7.439603
70	2.644451	77.463190	1.218955	7.586683
80	2.771413	89.164590	1.277478	8.732707
90	2.814167	93.355090	1.297185	9.143120

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