The Enumeration of Neighbors on Cubic and Hexagonal-Based Lattices

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(Manuscript received October 2, 1969)

Radii and occupation numbers have been calculated for the first 50 shells of neighbors on each atomic sublattice for the CsCl, NaCl, *zincblende, wurtzite, and* CaF_2 *binary lattices. We present the results in tabular form along with rules for extending the tables to higher shell numbers. A sublattice approach is used and tables are given for key cubic and hexagonal-based sublattices. The generality of the sublattice approach is such as to allow easy application of the tables to more complex lattice structures or to such problems as enumeration of preferred interstitial sites. A number-theoretic explanation is offered for previously observed difficulties in obtaining a simple expression for the radius of the m-th shell in cubic-based structures.*

I. INTRODUCTION

In discussing phenomena involving the interaction of ions in a crystalline lattice it is often necessary to know the radii and occupation numbers of near-lying shells of lattice sites. Such information is extremely important, for example, in the interpretation of donor-acceptor pair recombination spectra[1,2] and in calculations of ion pairing[3,4] and other defect clustering phenomena. The present work was motivated by the apparent lack of any generally available tables or formulae for calculating these m-th neighbor shell parameters for common lattices. Shell radius formulae and partial tables have been published[1,2] for the interpretation of pair spectra in materials with zincblende lattices but these tables are inadequate for other applications. Wood[5] and Ferris-Prabhu[6] have given slightly more complete treatments but do not present sufficiently general rules to allow indefinite extension of their tables.* The methods which will be described here differ from those

* In fact, if the diamond lattice radius rules given by Ferris-Prabhu[6] were used to extend his table beyond the 25 shells which he lists, one would err in predicting the radius of the 28th shell and would have all higher shells improperly numbered. Further errors would be made for much higher shell numbers.

reported previously[1,2,5,6] in that greater attention is given to the formulation of general rules which allow extension of the tables to higher shell numbers. It is hoped, however, that the tables presented will be sufficiently large for most applications and will not require extension. The general approach will be discussed in Section II and final tables of shell parameters will be presented together in Section III.

II. DISCUSSION

The notation to be used throughout is as follows: A convenient lattice point will be chosen as the origin and will be taken as the center of a spherical shell which is allowed to expand. At certain radii, ρ_m , the shell will coincide with other points of the lattice. The number, Z_m , of lattice points on the shell of radius ρ_m will be referred to as the occupation number of the m-th shell or the number of m-th neighbors. To find the radius and occupation number of the m-th shell, the following general approach[5,6] will be used: For each lattice a rectangular set of basis vectors ($\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$) will be chosen in such a way as to allow the coordinates of any lattice point to be written as (ℓ_1 , ℓ_2 , ℓ_3) where the ℓ_i are integers. All lattice points will therefore fall on the corners of rectangular parallelepiped (usually cubic) cells of the basis lattice but since the basis lattice is smaller than the actual lattice, there will be sets of integers which do not correspond to actual lattice points. Rules must therefore be formulated to allow these fictitious points to be rejected in the enumeration process. Points of the real lattice can then be enumerated by systematically counting all allowed combinations (ℓ_1 , ℓ_2 , ℓ_3). Since each point (ℓ_1 , ℓ_2 , ℓ_3) is located on a sphere of radius

$$\rho^2 = \ell_1^2 a_1^2 + \ell_2^2 a_2^2 + \ell_3^2 a_3^2 , \tag{1}$$

one can obtain Z_m by counting all lattice points with equal ρ^2 values and arranging the shells in order of ascending ρ^2. This process is simplified by making use of reflection and permutation symmetries but is best done by computer in any case.

It frequently turns out that one can write the radius of the m-th shell as a simple function of m: $\rho_m = f(m)$. Although there is no *a priori* reason to expect that such a formula will exist for any given lattice, it is very convenient if one can be found. (Radius formulae are useful, for example, in estimating the number of ℓ_i values which must be considered in order to count all lattice points of the m-th shell.) Since the subject of radius formulae has been a source of some confusion in the literature,[6] it will be given special attention in the discussions of specific lattices which follow.

2.1 *Cubic-Based Lattices*

Four monatomic cubic-based lattices will be considered first: Simple Cubic (sc), Body Centered Cubic (bcc), Edge Centered Cubic (ecc), and Face Centered Cubic (fcc). In each case the origin will be chosen to be at a cube corner and the basis vectors will be $(a/2)\mathbf{i}$, $(a/2)\mathbf{j}$, and $(a/2)\mathbf{k}$, where a is the length of a full cube edge and $\mathbf{i}$, $\mathbf{j}$, and $\mathbf{k}$ are unit vectors in the x, y, and z directions respectively which are taken to be cube edges. In the case of sc, one could choose vectors of length a but the $a/2$ choice turns out to be more convenient.

The bcc, fcc, and ecc lattices will each be decomposed into two sublattices: Sublattice 1 will consist of cube corners (as defined by the position of the origin) and sublattice 2 will consist of body centers (bc), face centers (fc), or edge centers (ec) as the case may be. This is illustrated in Fig. 1.

Since the basis lattice is a sc lattice with edge length $a/2$, all lattice points of the larger sc, fcc, ecc, and bcc structures can be written with integer coordinates (ℓ_1, ℓ_2, ℓ_3). Furthermore, it is seen by inspection that the following rules apply: (*i*) Points on sublattice 1 are obtained if and only if ℓ_1, ℓ_2, and ℓ_3 are all even. (*ii*) Points on the bc sublattice

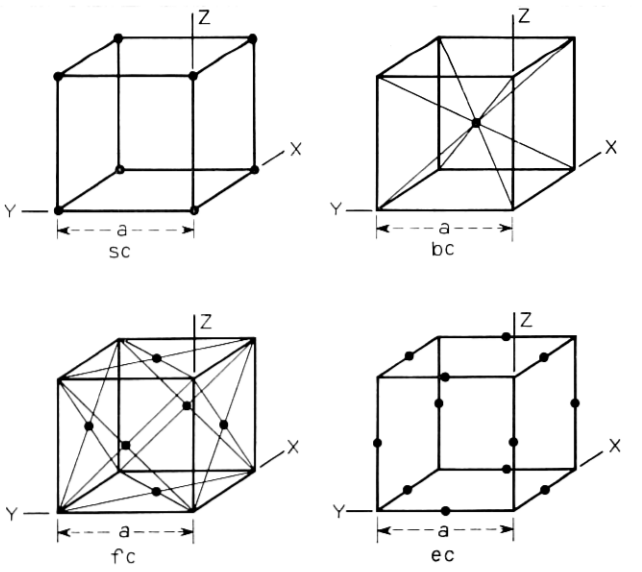

Fig. 1—The fundamental cubic-based lattices sc, bcc, fcc and ecc are shown decomposed into convenient sublattices: sc = sc, bcc = (bc + sc), fcc = (fc + sc), ecc = (ec + sc).

are reached if and only if the coordinates are all odd. (*iii*) Points on the fc sublattice are reached if and only if two of the coordinates are odd. (*iv*) Points on the ec sublattice are reached if and only if two of the coordinates are even.

By systematically enumerating all combinations of ℓ_1 , ℓ_2 , and ℓ_3 that satisfy these criteria, one obtains all points of the respective sublattices. For the simple lattices considered here one can make use of reflection symmetry and permutation symmetry by considering only points for which $\ell_1 \geqq \ell_2 \geqq \ell_3 \geqq 0$. Any point ($\ell_1$, ℓ_2 , ℓ_3) is then one-, three-, or sixfold degenerate under permutation of coordinates (p) and two-, four-, or eightfold degenerate under reflection in the coordinate planes (d). The total number of points equivalent to (ℓ_1 , ℓ_2 , ℓ_3) is then $Z_i = dp$ where d and p are given by Table I where A, B, and C are distinct integers and order is immaterial. In many cases there will be two or more nonequivalent sets of lattice points on the same shell. In such cases $Z_m = \sum_i d_i p_i$ where i ranges over the various distinguishable sets of lattice points. For example, the 22nd shell of the sc lattice has $\rho^2 = 100(a/2)^2$. This shell contains points of the type (8, 6, 0) and (10, 0, 0) (in units of $a/2$). There are $6 \times 4 = 24$ of the former and $3 \times 2 = 6$ of the latter for a total of 30 points on this shell.

Having chosen cartesian basis vectors of equal lengths we can write the distance from the origin to any lattice point in the form

$$r^2 = \ell_1^2 + \ell_2^2 + \ell_3^2 , \tag{2}$$

where r is the shell radius in units of the basis vector length. Thus the square of the radius vector to any lattice point must be expressible as the sum of three perfect squares. This is highly relevant to previously observed difficulties in obtaining simple expressions for the radius r_m of the m-th shell in cubic based lattices. The usual difficulty is that one is able to find a formula which works only for a limited number of

TABLE I—NUMBER OF POINTS EQUIVALENT BY SYMMETRY

Coordinates of the Form	p
(A, A, A)	1
(A, A, C)	3
(A, B, C)	6
Number of Zero Coordinates	d
2	2
1	4
0	8

TABLE II—VALUES OF r_m^2 WHICH ARE FORBIDDEN IN CUBIC-BASED LATTICES*

	r				
s	0	1	2	3	4
0	7	28	112	448	1792
1	15	60	240	960	·
2	23	92	368	·	·
3	31	124	·	·	·
4	39	156	·	·	·
5	47	188	·	·	·
6	55	220	·	·	
7	63	252	·		
8	71	·			
9	79	·			
10	87	·			
11	95	·			
12	103	·			
·	·				
·	·				

* Numbers of the form $4^r(8s + 7)$ where r and s are integers $\geqq 0$.

shells and then fails by predicting a shell of lattice points at some radius r_m where, in fact, no actual lattice points exist. Thomas, and others,[1,2] call these "empty shells" and count them as m-th neighbors with $Z_m = 0$. Through this device a formula can be made to work for all r_m. Thomas, and others, also give a formula which predicts the shells which will require $Z_m = 0$ for the zincblende lattice but do not discuss the origin of this formula. In every case investigated in the present work, a failure of shell radius formulae occurred because these formulae predicted values for r_i^2 which were not expressible as the sum of three perfect squares.* It is known from the theory of numbers[7] that an integer can be expressed as the sum of three squares† if and only if it is not of the form $4^r(8s + 7)$ where r and s are integers $\geqq 0$. Thus whenever a radius formula predicts a value of r_m^2 of the form $4^r(8s + 7)$, no shell of lattice points will exist since r_m^2 will fail to satisfy the physical constraint given by equation (2). A few of these forbidden r_m^2 values are listed in Table II.

The sc, bc, fc, and ec sublattices form a basic set from which one can construct more complex lattices. They all have reflection and per-

* It is possible, in more complex lattices, for a radius rule to fail for other reasons.

† It can be shown that *any* integer can be expressed as the sum of not more than four squares, nine cubes, or nineteen fourth powers.[7] The important point, however, is that three squares are sufficient.

mutation symmetry, however, and will not be directly applicable to any lattices or sublattices that do not share these symmetries. This is illustrated in the final monatomic lattice to be considered in this section: diamond.

The diamond lattice is composed of two interpenetrating fcc lattices which are shifted along a common diagonal by an amount $(a/4, a/4, a/4)$ as indicated in Fig. 2. A corner of one of these fcc lattices will be chosen as the origin and this sublattice will be denoted "I." The shifted sublattice is then "II." The basis vectors are taken to be $a/4$ in length and span a sc basis lattice with cube edges $a/4$. The restrictions on ℓ_1, ℓ_2, ℓ_3 are found by inspection (this process is aided by consideration of projections in the coordinate planes), and are given in Table III along with a summary of similar results for the sc, bc, fc, and ec sublattices. The radius formulae given in column 5 of Table III are obtained by inserting general integers of the forms given in column 4

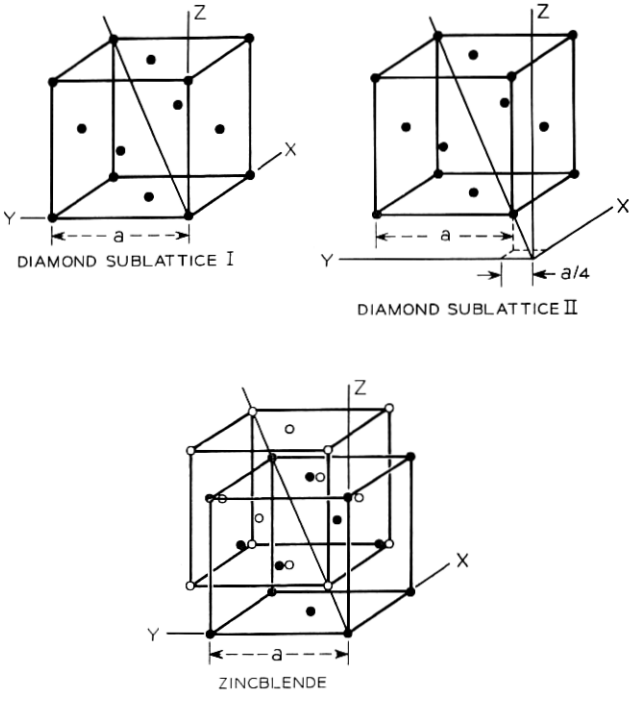

Fig. 2—The diamond and zincblende lattices are shown decomposed into two fcc sublattices. In diamond, atoms on sublattices I and II are identical. In zincblende, atoms on I are of one type and atoms on II are the other type.

TABLE III—SUMMARY OF THE FUNDAMENTAL CUBIC-BASED MONATOMIC SUBLATTICES

Lattice	Sublattice	Basis vectors chosen	Conditions on Coordinate Integers (ℓ_1, ℓ_2, ℓ_3)	r_m^2	Units of r_m^2	Notes
sc	sc (cube corners)	$(a/2)\mathbf{i}$, $(a/2)\mathbf{j}$, $(a/2)\mathbf{k}$	ℓ_1, ℓ_2, ℓ_3 all even	$r_m^2 = 4(m + n)$	$(a/2)^2$	a, b
bcc	bc (body centers)	$(a/2)\mathbf{i}$, $(a/2)\mathbf{j}$, $(a/2)\mathbf{k}$	ℓ_1, ℓ_2, ℓ_3 all odd	$r_m^2 = (8m - 5)$	$(a/2)^2$	a, c
fcc	fc (face centers)	$(a/2)\mathbf{i}$, $(a/2)\mathbf{j}$, $(a/2)\mathbf{k}$	exactly two of ℓ_1, ℓ_2, ℓ_3 must be odd	$r_m^2 = 2(2m - 1)$	$(a/2)^2$	a, c
ecc	ec (edge centers)	$(a/2)\mathbf{i}$, $(a/2)\mathbf{j}$, $(a/2)\mathbf{k}$	exactly two of ℓ_1, ℓ_2, ℓ_3 must be even	$r_m^2 = (4m - 3)$	$(a/2)^2$	a, c
diamond	I (unshifted fcc lattice)	$(a/4)\mathbf{i}$, $(a/4)\mathbf{j}$, $(a/4)\mathbf{k}$	ℓ_1, ℓ_2, ℓ_3 all even $\ell_1 + \ell_2 + \ell_3$ of the form $4s$	$r_m^2 = 8(m + n)$	$(a/4)^2$	a, b, d
diamond	II (fcc lattice shifted by $(a/4, a/4, a/4)$)	$(a/4)\mathbf{i}$, $(a/4)\mathbf{i}$, $(a/4)\mathbf{k}$	ℓ_1, ℓ_2, ℓ_3 all odd $\ell_1 + \ell_2 + \ell_3$ of the form $4s - 1$	$r_m^2 = (8m - 5)$	$(a/4)^2$	a, c

a. In the r_m^2 column m is an index numbering shells of neighbors *within each sublattice.*
b. n is an integer which starts at 0 and is incremented by 1 every time the formula (including previous increments) predicts an r_m^2 value of the form $4^r(8s + 7)$ where r and s are integers ≥ 0. (See also Table II and discussion in text.)
c. The radius formula in this case never predicts any r_m^2 values of the forbidden form $4^r(8s + 7)$.
d. Alternatively the sc and fc sublattices can be combined and used directly by multiplying the r_m^2 values of the fcc sublattices by 4 to convert to the $a/4$ basis chosen for diamond.

into equation (2) and identifying "m" in the resulting expression.

The diamond sublattice I can be worked out directly using the rules given in Table III or can be formed from the results of sc and fc by converting the r^2 values from the $a/2$ basis to the $a/4$ basis, interleaving the sc and fc sublattices to form a full fcc lattice, and renumbering the shells. The renumbering of shells invalidates the previous r_m^2 formulae but a new formula is found for the full fcc lattice. The diamond sublattice II enumeration proceeds in a straightforward manner but requires explicit counting of a greater number of points since there is less conveniently useable symmetry. In this case none of the simpler sublattices can be used directly since diamond II lacks the full cubic symmetries.

The simple monatomic lattices and sublattices can now be combined to describe physically interesting binary crystals. We adopt the following notation for sublattices of binary crystals: One X atom of the compound X_mY_n is chosen to lie at the origin and all other X atoms are said to occupy sublattice I_X. Sublattice II_X consists of all Y atoms when X is at the origin. Similarly, if Y is at the origin then Y atoms occupy sublattice I_Y and X atoms occupy II_Y. The distinction between I_X and I_Y or II_X and II_Y disappears for compounds of the type X_mY_m where all atoms of X and Y could be interchanged without any physically observable effect. The zincblende lattice, shown in the lower portion of Fig. 2, differs from diamond only in that sublattices I and II are occupied by different atomic species. Figure 3 shows three more commonly observed binary lattices: NaCl, CsCl, and CaF_2. In Table IV we show how these lattices can be formed from the basic cubic sublattices. Thus, for example, a table of r_m^2 and Z_m values for NaCl sublattice I (Na neighbors if Na is at the origin or Cl neighbors if Cl is at the origin) is composed of values from the sc and fc tables arranged in order of increasing r_m^2. The NaCl II sublattice is obtained by combining the bc and ec sublattices. All final tables of r_m^2 and Z_m will be given in Section III.

2.2 *Hexagonal-Based Lattices*

The hexagonal based lattices to be considered here are: (*i*) monatomic hexagonal close-packed (hcp) and (*ii*) wurtzite. These lattices are pictured in Fig. 4 along with a diagram of the basal plane showing how the basis vectors are chosen. The origin is placed at a corner of the hexagonal prism and the z-axis is taken along the c-axis of the crystal. The x and y axes are chosen as shown in Fig. 4 and the basis vectors are $(a/2)\mathbf{i}$, $[a/2(3)^{\frac{1}{2}}]\mathbf{j}$, $[2a/(6)^{\frac{1}{2}}]\mathbf{k}$. We assume that the hcp structure is the

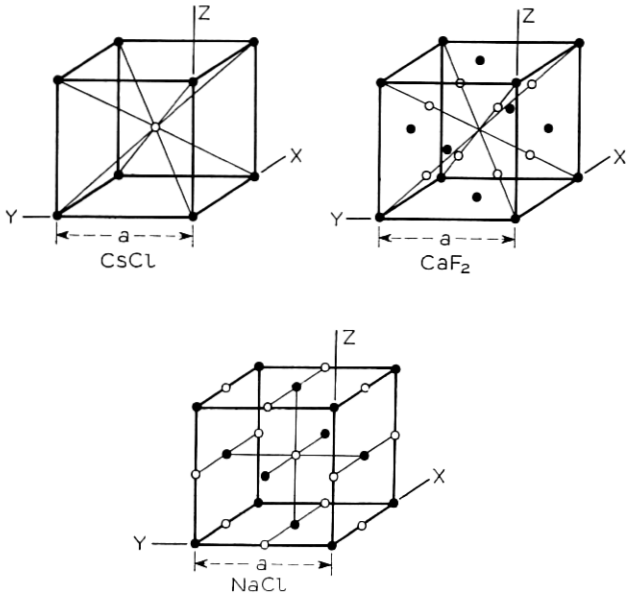

Fig. 3—The cubic-based binary lattices CsCl, NaCl, and CaF_2. CaF_2 is shown with Ca at the origin.

"ideal" one obtained by closest packing of spheres. In this case $c = (8/3)^{\frac{1}{2}}a$. The wurtzite structure is composed of two such hcp sublattices displaced along their common c-axis by an amount $u = (3/8)c$ and having atoms of different types occupying the two hcp sublattices. The unshifted sublattice will be called I and the shifted sublattice will be II. The enumeration of neighbors proceeds as in the cases already discussed and need not be detailed again. By inspection of the planes of lattice points one can obtain[5] the following conditions for ℓ_1 , ℓ_2 , and ℓ_3 for the hcp lattice:

$$\frac{3\ell_1 - \ell_2 + (-1)^{\ell_3} - 1}{6} = \text{integer}. \tag{3}$$

To identify points of the wurtzite II sublattice one can first locate points of the hcp lattice (wurtzite I) using equation (3) and then add $(\frac{3}{8})c$ to their z coordinates. The r_m^2 values are not integers for hcp and wurtzite because the separations between x-, y-, and z-planes of atoms are not related by rational numbers. Thus no $r_m^2 = f(m)$ formulae are expected. The radii are related to the coordinate integers by the follow-

TABLE IV—DECOMPOSITION OF CUBIC-BASED BINARY LATTICES INTO FUNDAMENTAL SUBLATTICES

Lattice	Sublattice	Basis Vectors	Equivalent Monatomic Lattice
NaCl	I Same as ion at origin	(a/2)i, (a/2)j, (a/2)k	fcc (sc + fc)
	II Opposite from ion at origin	(a/2)i, (a/2)j, (a/2)k	fcc shifted by (a/2, 0, 0) or (ec + bc)
CsCl	I Same	(a/2)i, (a/2)j, (a/2)k	sc
	II Opposite	(a/2)i, (a/2)j, (a/2)k	bc
Zincblende	I Same	(a/4)i, (a/4)j, (a/4)k	diamond I
	II Opposite	(a/4)i, (a/4)j, (a/4)k	diamond II
CaF_2	Ca Sublattice I_A Ca at orgin	(a/4)i, (a/4)j, (a/4)k	diamond I
	F Sublattice II_A Ca at origin	(a/4)i, (a/4)j, (a/4)k	bc with cube edge $a/2$
	F Sublattice I_B F at origin	(a/4)i, (a/4)j, (a/4)k	sc
	Ca Sublattice II_B F at origin	(a/4)i, (a/4)j, (a/4)k	diamond II

ing formulae

$$r^2 = \frac{3\ell_1^2 + \ell_2^2 + 8\ell_3^2}{12} \text{ (hcp)} \tag{4}$$

and

$$r^2 = \frac{6\ell_1^2 + 2\ell_2^2 + (4\ell_3 + 3)^2}{24} \text{ (wurtzite II)}. \tag{5}$$

III. TABLES

Tables V–VIII contain shell parameters for the basic monatomic lattices and sublattices. Table VIII can be used for both diamond and zincblende. In each case the shell number m refers to the m-th shell of neighbors *on that sublattice*. In order to combine two or more sublattices one must convert the r_m^2 values to the same basis (a, $a/2$, $a/4$, and so on) and interweave the appropriate columns in order of increasing r^2. The sc table includes r_m^2 columns for three choices of basis vector lengths:

a, $a/2$ and $a/4$. Tables IX–XIII give the corresponding results for CsCl, NaCl, CaF_2 and wurtzite.

The cubic based tables are easily extended to higher shell number by using the methods described earlier. In this regard the shell radius formulae are particularly useful if the search for lattice points is done by hand. For the diamond II and hexagonal based lattices, however, one must resort to computer enumeration and summation of allowed combinations of coordinates.

It should be pointed out here that there is a possible complication which can arise in utilizing these tables in physical applications involving more complex lattices. As was indicated in Section II, many of the shells in Tables V–XIII are degenerate. Although points on the same shell always belong to the same sublattice (for all sublattices which have been defined here), it is possible in some cases that different points

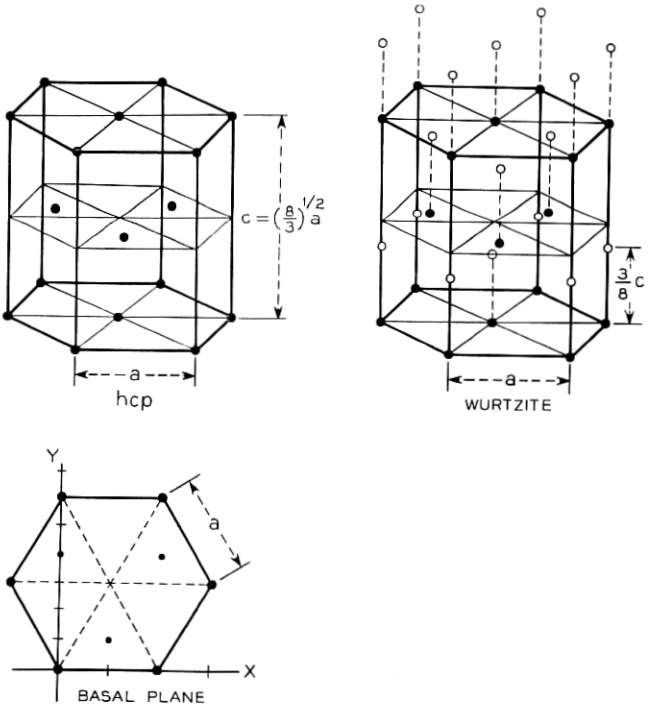

Fig. 4—Geometry of the hcp and wurtzite lattices. Wurtzite consists of two hcp lattices shifted $\frac{3}{8}c$ along their common c axis. The two hcp sublattices of wurtzite are occupied by different atomic species. $\mathbf{x} = (a/2)\mathbf{i}$; $\mathbf{y} = [a/2(3)^{1/2}]\mathbf{j}$; $\mathbf{z} = [2a/(6)^{1/2}\mathbf{k} = (c/2)\mathbf{k}$.

TABLE V—SHELL PARAMETERS FOR THE SC LATTICES*

Shell	$r^2(a^2)$	$r^2(a^2/4)$	$r^2(a^2/16)$	Z
1 (1)†	1	4	16	6
2 (2)	2	8	32	12
3 (3)	3	12	48	8
4 (4)	4	16	64	6
5 (5)	5	20	80	24
6 (6)	6	24	96	24
7 (8)	8	32	128	12
8 (9)	9	36	144	30
9 (10)	10	40	160	24
10 (11)	11	44	176	24
11 (12)	12	48	192	8
12 (13)	13	52	208	24
13 (14)	14	56	224	48
14 (16)	16	64	256	6
15 (17)	17	68	272	48
16 (18)	18	72	288	36
17 (19)	19	76	304	24
18 (20)	20	80	320	24
19 (21)	21	84	336	48
20 (22)	22	88	352	24
21 (24)	24	96	384	24
22 (25)	25	100	400	30
23 (26)	26	104	416	72
24 (27)	27	108	432	32
25 (29)	29	116	464	72
26 (30)	30	120	480	48
27 (32)	32	128	512	12
28 (33)	33	132	528	48
29 (34)	34	136	544	48
30 (35)	35	140	560	48
31 (36)	36	144	576	30
32 (37)	37	148	592	24
33 (38)	38	152	608	72
34 (40)	40	160	640	24
35 (41)	41	164	656	96
36 (42)	42	168	672	48
37 (43)	43	172	688	24
38 (44)	44	176	704	24
39 (45)	45	180	720	72
40 (46)	46	184	736	48
41 (48)	48	192	768	8
42 (49)	49	196	784	54
43 (50)	50	200	800	84
44 (51)	51	204	816	48
45 (52)	52	208	832	24
46 (53)	53	212	848	72
47 (54)	54	216	864	96
48 (56)	56	224	896	48
49 (57)	57	228	912	48
50 (58)	58	232	928	24

* For convenience, r^2 has been given for three choices of basis-vector lengths [a^2, $(a/2)^2$, and $(a/4)^2$].

† Numbers in parentheses conform to the notation of Refs. 1 and 2 in which "missing shells" are included in the sequential numbering as discussed in the text. If these shell numbers are used one must set $n = 0$ in the radius formula.

TABLE VI—SHELL PARAMETERS FOR THE BC AND EC SUBLATTICES*

Shell	bc Sublattice		ec Sublattice	
	r^2	Z	r^2	Z
1	3	8	1	6
2	11	24	5	24
3	19	24	9	30
4	27	32	13	24
5	35	48	17	48
6	43	24	21	48
7	51	48	25	30
8	59	72	29	72
9	67	24	33	48
10	75	56	37	24
11	83	72	41	96
12	91	48	45	72
13	99	72	49	54
14	107	72	53	72
15	115	48	57	48
16	123	48	61	72
17	131	120	65	96
18	139	72	69	96
19	147	56	73	48
20	155	96	77	96
21	163	24	81	102
22	171	120	85	48
23	179	120	89	144
24	187	48	93	48
25	195	96	97	48
26	203	96	101	168
27	211	72	105	96
28	219	96	109	72
29	227	120	113	96
30	235	48	117	120
31	243	104	121	78
32	251	168	125	144
33	259	96	129	144
34	267	48	133	48
35	275	120	137	96
36	283	72	141	96
37	291	96	145	96
38	299	192	149	168
39	307	72	153	144
40	315	144	157	72
41	323	96	161	192
42	331	72	165	96
43	339	144	169	78
44	347	120	173	168
45	355	96	177	48
46	363	104	181	120
47	371	192	185	192
48	379	72	189	192
49	387	120	193	48
50	395	192	197	120

* r^2 is in units of $(a/2)^2$.

TABLE VII—SHELL PARAMETERS FOR THE FC AND HCP SUBLATTICES*

Shell	fc Sublattice		hcp Lattice	
	r^2	Z	r^2	Z
1	2	12	1.00	12
2	6	24	2.00	6
3	10	24	2.67	2
4	14	48	3.00	18
5	18	36	3.67	12
6	22	24	4.00	6
7	26	72	5.00	12
8	30	48	5.67	12
9	34	48	6.00	6
10	38	72	6.33	6
11	42	48	6.67	12
12	46	48	7.00	24
13	50	84	7.33	6
14	54	96	8.33	12
15	58	24	9.00	12
16	62	96	9.67	24
17	66	96	10.00	12
18	70	48	10.33	12
19	74	120	10.67	2
20	78	48	11.00	12
21	82	48	11.33	6
22	86	120	11.67	24
23	90	120	12.00	6
24	94	96	12.33	12
25	98	108	13.00	24
26	102	48	13.67	12
27	106	72	14.33	6
28	110	144	14.67	24
29	114	96	15.00	12
30	118	72	15.33	12
31	122	120	15.67	24
32	126	144	16.00	6
33	130	48	16.33	12
34	134	168	17.00	24
35	138	96	17.67	24
36	142	48	18.00	18
37	146	192	18.33	12
38	150	120	18.67	12
39	154	96	19.00	24
40	158	96	19.67	12
41	162	120	20.33	12
42	166	120	21.00	36
43	170	144	21.67	24
44	174	144	22.00	12
45	178	96	22.33	18
46	182	144	22.67	12
47	186	144	23.00	24
48	190	48	23.33	12
49	194	240	23.67	48
50	198	120	24.00	2

* For the fc sublattices r^2 is in units of $(a/2)^2$. For hcp r^2 is expressed in units of a^2.

TABLE VIII—SHELL PARAMETERS FOR SUBLATTICES OF THE DIAMOND OR ZINCBLENDE LATTICES*

Shell	Sublattice I		Sublattice II	
	r^2	Z	r^2	Z
1 (1)†	8	12	3	4
2 (2)	16	6	11	12
3 (3)	24	24	19	12
4 (4)	32	12	27	16
5 (5)	40	24	35	24
6 (6)	48	8	43	12
7 (7)	56	48	51	24
8 (8)	64	6	59	36
9 (9)	72	36	67	12
10 (10)	80	24	75	28
11 (11)	88	24	83	36
12 (12)	96	24	91	24
13 (13)	104	72	99	36
14 (15)	120	48	107	36
15 (16)	128	12	115	24
16 (17)	136	48	123	24
17 (18)	144	30	131	60
18 (19)	152	72	139	36
19 (20)	160	24	147	28
20 (21)	168	48	155	48
21 (22)	176	24	163	12
22 (23)	184	48	171	60
23 (24)	192	8	179	60
24 (25)	200	84	187	24
25 (26)	208	24	195	48
26 (27)	216	96	203	48
27 (28)	224	48	211	36
28 (29)	232	24	219	48
29 (31)	248	96	227	60
30 (32)	256	6	235	24
31 (33)	264	96	243	52
32 (34)	272	48	251	84
33 (35)	280	48	259	48
34 (36)	288	36	267	24
35 (37)	296	120	275	60
36 (38)	304	24	283	36
37 (39)	312	48	291	48
38 (40)	320	24	299	96
39 (41)	328	48	307	36
40 (42)	336	48	315	72
41 (43)	344	120	323	48
42 (44)	352	24	331	36
43 (45)	360	120	339	72
44 (47)	376	96	347	60
45 (48)	384	24	355	48
46 (49)	392	108	363	52
47 (50)	400	30	371	96
48 (51)	408	48	379	36
49 (52)	416	72	387	60
50 (53)	424	72	395	96

* r^2 is in units of $(a/4)^2$.

† Numbers in parentheses apply *only* to sublattice I and conform to the notation of Refs. 1 and 2 in which "missing shells" are included in the sequential numbering as discussed in the text. If these shell numbers are used one must set $n = 0$ in the radius formula.

TABLE IX—SHELL PARAMETERS FOR SUBLATTICES OF THE CsCl LATTICE*

Shell	Sublattice I		Sublattice II	
	r^2	Z	r^2	Z
1	4	6	3	8
2	8	12	11	24
3	12	8	19	24
4	16	6	27	32
5	20	24	35	48
6	24	24	43	24
7	32	12	51	48
8	36	30	59	72
9	40	24	67	24
10	44	24	75	56
11	48	8	83	72
12	52	24	91	48
13	56	48	99	72
14	64	6	107	72
15	68	48	115	48
16	72	36	123	48
17	76	24	131	120
18	80	24	139	72
19	84	48	147	56
20	88	24	155	96
21	96	24	163	24
22	100	30	171	120
23	104	72	179	120
24	108	32	187	48
25	116	72	195	96
26	120	48	203	96
27	128	12	211	72
28	132	48	219	96
29	136	48	227	120
30	140	48	235	48
31	144	30	243	104
32	148	24	251	168
33	152	72	259	96
34	160	24	267	48
35	164	96	275	120
36	168	48	283	72
37	172	24	291	96
38	176	24	299	192
39	180	72	307	72
40	184	48	315	144
41	192	8	323	96
42	196	54	331	72
43	200	84	339	144
44	204	48	347	120
45	208	24	355	96
46	212	72	363	104
47	216	96	371	192
48	224	48	379	72
49	228	48	387	120
50	232	24	395	192

* r^2 is in units of $(a/2)^2$.

TABLE X—SHELL PARAMETERS FOR SUBLATTICES OF THE NaCl LATTICE*

Shell	Sublattice I		Sublattice II	
	r^2	Z	r^2	Z
1	2	12	1	6
2	4	6	3	8
3	6	24	5	24
4	8	12	9	30
5	10	24	11	24
6	12	8	13	24
7	14	48	17	48
8	16	6	19	24
9	18	36	21	48
10	20	24	25	30
11	22	24	27	32
12	24	24	29	72
13	26	72	33	48
14	30	48	35	48
15	32	12	37	24
16	34	48	41	96
17	36	30	43	24
18	38	72	45	72
19	40	24	49	54
20	42	48	51	48
21	44	24	53	72
22	46	48	57	48
23	48	8	59	72
24	50	84	61	72
25	52	24	65	96
26	54	96	67	24
27	56	48	69	96
28	58	24	73	48
29	62	96	75	56
30	64	6	77	96
31	66	96	81	102
32	68	48	83	72
33	70	48	85	48
34	72	36	89	144
35	74	120	91	48
36	76	24	93	48
37	78	48	97	48
38	80	24	99	72
39	82	48	101	168
40	84	48	105	96
41	86	120	107	72
42	88	24	109	72
43	90	120	113	96
44	94	96	115	48
45	96	24	117	120
46	98	108	121	78
47	100	30	123	48
48	102	48	125	144
49	104	72	129	144
50	106	72	131	120

* r^2 is in units of $(a/2)^2$.

TABLE XI—SHELL PARAMETERS FOR SUBLATTICES OF THE CaF_2 LATTICE WHEN Ca IS TAKEN TO BE AT THE ORIGIN*

Shell	Sublattice I_{Ca}		Sublattice II_{Ca}	
	r^2	Z	r^2	Z
1	8	12	3	8
2	16	6	11	24
3	24	24	19	24
4	32	12	27	32
5	40	24	35	48
6	48	8	43	24
7	56	48	51	48
8	64	6	59	72
9	72	36	67	24
10	80	24	75	56
11	88	24	83	72
12	96	24	91	48
13	104	72	99	72
14	120	48	107	72
15	128	12	115	48
16	136	48	123	48
17	144	30	131	120
18	152	72	139	72
19	160	24	147	56
20	168	48	155	96
21	176	24	163	24
22	184	48	171	120
23	192	8	179	120
24	200	84	187	48
25	208	24	195	96
26	216	96	203	96
27	224	48	211	72
28	232	24	219	96
29	248	96	227	120
30	256	6	235	48
31	264	96	243	104
32	272	48	251	168
33	280	48	259	96
34	288	36	267	48
35	296	120	275	120
36	304	24	283	72
37	312	48	291	96
38	320	24	299	192
39	328	48	307	72
40	336	48	315	144
41	344	120	323	96
42	352	24	331	72
43	360	120	339	144
44	376	96	347	120
45	384	24	355	96
46	392	108	363	104
47	400	30	371	192
48	408	48	379	72
49	416	72	387	120
50	424	72	395	192

* r^2 is in units of $(a/4)^2$.

TABLE XII—SHELL PARAMETERS FOR SUBLATTICES OF THE CaF_2 LATTICE WHEN F IS TAKEN TO BE AT THE ORIGIN*

Shell	Sublattice I_F		Sublattice II_F	
	r^2	Z	r^2	Z
1	4	6	3	4
2	8	12	11	12
3	12	8	19	12
4	16	6	27	16
5	20	24	35	24
6	24	24	43	12
7	32	12	51	24
8	36	30	59	36
9	40	24	67	12
10	44	24	75	28
11	48	8	83	36
12	52	24	91	24
13	56	48	99	36
14	64	6	107	36
15	68	48	115	24
16	72	36	123	24
17	76	24	131	60
18	80	24	139	36
19	84	48	147	28
20	88	24	155	48
21	96	24	163	12
22	100	30	171	60
23	104	72	179	60
24	108	32	187	24
25	116	72	195	48
26	120	48	203	48
27	128	12	211	36
28	132	48	219	48
29	136	48	227	60
30	140	48	235	24
31	144	30	243	52
32	148	24	251	84
33	152	72	259	48
34	160	24	267	24
35	164	96	275	60
36	168	48	283	36
37	172	24	291	48
38	176	24	299	96
39	180	72	307	36
40	184	48	315	72
41	192	8	323	48
42	196	54	331	36
43	200	84	339	72
44	204	48	347	60
45	208	24	355	48
46	212	72	363	52
47	216	96	371	96
48	224	48	379	36
49	228	48	387	60
50	232	48	395	96

* r^2 is in units of $(a/4)^2$.

TABLE XIII—SHELL PARAMETERS FOR SUBLATTICES OF THE WURTZITE LATTICE*

Shell	Sublattice I		Sublattice II	
	r^2	Z	r^2	Z
1	1.000	12	.375	4
2	2.000	6	1.042	1
3	2.667	2	1.375	9
4	3.000	18	2.042	6
5	3.667	12	2.375	9
6	4.000	6	3.375	9
7	5.000	12	3.708	3
8	5.667	12	4.042	6
9	6.000	6	4.375	18
10	6.333	6	4.708	3
11	6.667	12	5.042	7
12	7.000	24	5.375	3
13	7.333	6	5.708	6
14	8.333	12	6.042	6
15	9.000	12	6.375	12
16	9.667	24	7.042	1
17	10.000	12	7.375	15
18	10.333	12	7.708	6
19	10.667	2	8.042	24
20	11.000	12	8.375	9
21	11.333	6	8.708	3
22	11.667	24	9.042	6
23	12.000	6	9.375	12
24	12.333	12	9.708	9
25	13.000	24	10.042	12
26	13.667	12	10.375	9
27	14.333	6	10.708	3
28	14.667	24	11.042	6
29	15.000	12	11.375	6
30	15.333	12	11.708	9
31	15.667	24	12.042	12
32	16.000	6	12.375	21
33	16.333	12	12.708	6
34	17.000	24	13.042	6
35	17.667	24	13.375	15
36	18.000	18	13.708	12
37	18.333	12	14.042	30
38	18.667	12	14.375	18
39	19.000	24	14.708	3
40	19.667	12	15.042	1
41	20.333	12	15.708	12
42	21.000	38	16.042	12
43	21.667	24	16.375	27
44	22.000	12	17.042	12
45	22.333	18	17.375	9
46	22.667	12	17.708	9
47	23.000	24	18.042	18
48	23.333	12	18.375	16
49	23.667	48	18.708	6
50	24.000	2	19.042	12

* r^2 is in units of a^2.

on the same shell can occupy physically distinguishable sites in the lattice (that is, sites which, even though they belong to the same sublattice, have differing local environments). In addition to this, interactions between electrons and holes bound to donors and acceptors may depend upon the relative orientations of the electron and hole wavefunctions, the vector separation between ions, and the crystallographic axes. Thus in the interpretation of pair spectra, for example, one may expect energy splittings in such cases to cause deviations from the spacings and magnitudes predicted on the basis of neighbor tables.[1,2,8,9] Wurtzite is particularly complicated in this respect, providing a variety of local symmetries for donor-acceptor pairs involving substitutional and/or interstitial ions.[9,10] In the absence of externally imposed asymmetries, however, lattice sites on the same sublattice will usually be physically indistinguishable. Among the structures considered here, wurtzite is the sole exception. For this reason it was felt that the tables would be unnecessarily complicated by the inclusion of any information regarding degeneracies or coordinate types. In most cases, however, the computer programs were written in such a way as to preserve this information and it is available from the authors upon request.

IV. FURTHER APPLICATIONS

The crystal structures which have been explicitly discussed account for the vast majority of binary compounds $X_M Y_N$ and virtually all of the important XY compounds. This is indicated in Table XIV where we have shown the crystal structures of the common binary compounds formed by combining elements from groupings IA, IIA, and IB–IVB* with elements from groups IVB–VIIB.[11] In Table XIV the important elemental and compound semiconductors, the oxides and chalcogenides of group IIA and IIB metals, the alkali halides, and the noble metal salts have been enclosed in heavy lines. It is seen that nearly all of these compounds crystallize in one of the structures which has been treated here. Furthermore, it is noted that many of the structures which were not treated explicitly are cubic-based or hexagonal-based so that the one might be able to utilize one or more of the basic sublattices calculated here.

In certain kinds of defect interaction calculations it may also be convenient to know the distribution of available interstitial sites as a function of distance from a given ion. Inspection of crystalline lattice

* The A and B notation used here for subgroups of the periodic table was chosen to agree with Frederikse[11] but is not uniform throughout the literature.

structures shows the most of them have regular arrays of preferred interstitial sites. These sites form a sublattice which can be treated by the methods already discussed. As an example we list in Table XV the first 25 shells of interstitial sites for the fcc lattice. These are at ec and bc sites. This table is the same as the table for Type III pair spectra given by Ryan and Miller.[2] Similar tables can be constructed for interstitials in other lattices.

V. SUMMARY

We have described a general method for obtaining radii and occupation numbers of m-th order shells of neighboring lattice points for cubic and hexagonal based lattices. The method described here will, in

TABLE XIV—A SUMMARY OF INORGANIC BINARY COMPOUNDS $X_M Y_N$ AND THEIR CRYSTAL STRUCTURES*

		Y		
X	IVB C, Si, Ge, Sn, Pb	VB N, P, As, Sb	VIB O, S, Se, Te	VIIB F, Cl, Br, I
IVB C, Si, Ge, Sn, Pb	X, SiC 3,7	XY, X_3Y_2 1,8	XY, XY_2 1,4,6,7,8	XY_4 6,8
IIIB B, Al, Ga, In	—	XY 3,4	X_2Y_3 3,4,6,7	—
IIB Zn, Cd, Hg	—	X_3Y_2 6,7,8	XY 1,3,4	XY_2 5,6,7,8
IB Cu, Ag, Au	—	X_3Y, XY_2, X_2Y 6,7,8	XY, X_2Y, XY_2 1,2,5,6,7,8	XY 1,3,4
IA Li, Na, K, Rb, Cs	—	—	X_2Y 5	XY 1,2
IIA Be, Mg, Ca, Sr, Ba	X_2Y 5,7,8	X_3Y_2 6,7	XY 1,3,4	XY_2 5,6,7,8

1. NaCl Structure
2. CsCl Structure
3. Zincblende Structure (Diamond in case of element)
4. Wurtzite Structure
5. CaF_2 Structure
6. Other Cubic-based Structure
7. Other Hexagonal-based Structure
8. Complex

* Roman numerals and A or B refer to groups and subgroups of the periodic table in the notation of Ref. 11. Only representative compound-types are indicated and not all of the elements of any one group form in all of the combinations shown. See Ref. 11 for an extensive list of specific compounds.

TABLE XV—THE FIRST 25 SHELLS OF PREFERRED INTERSTITIAL SITES FOR THE FCC LATTICE*

Shell	Interstitials	
	r^2	Z
1 (0)†	1	6
2 (1)	3	8
3 (2)	5	24
4 (4)	9	30
5 (5)	11	24
6 (6)	13	24
7 (8)	17	48
8 (9)	19	24
9 (10)	21	48
10 (12)	25	30
11 (13)	27	32
12 (14)	29	72
13 (16)	33	48
14 (17)	35	48
15 (18)	37	24
16 (20)	41	96
17 (21)	43	24
18 (22)	45	72
19 (24)	49	54
20 (25)	51	48
21 (26)	53	72
22 (28)	57	48
23 (29)	59	72
24 (30)	61	72
25 (32)	65	96

* This table was obtained by combining the first few shells of the bc and ec tables and is easily extended further. All r^2 values are in units of $(a/2)^2$.

† Numbers in parentheses conform to the notation of Refs. 1 and 2 in which "missing shells" are included in the sequential numbering as discussed in the text. Note that Ryan and Miller began the numbering with $m = 0$.

principle, work for *any* specific lattice if the basis vectors are properly chosen but is practical only in cases where the lattice contains no arbitrary angles or spacings. A general hexagonal lattice, for example, has an arbitrary c/a ratio which must be fixed before the basis vectors can be chosen. The principal results are contained in Tables V–XIII which contain shell parameters for simple building-block sublattices as well as physically interesting binary lattices. Extension of the tables to higher shell numbers and application of the tables to physical problems were discussed.

VI. ACKNOWLEDGMENTS

The authors would like to thank M. DiDomenico, Jr., for offering several helpful observations. We have also benefited from discussions with M. L. Howe and L. C. Luther.

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