



CRYSTALLINE ACCOMMODATION LAW EXPLAINS THE CRYSTALLINE STRUCTURE OF MATERIALS

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ABSTRACT

All crystalline materials crystallize in one of seven crystalline systems which have different shapes and sizes. Why crystalline materials take particular forms of crystals and what make the atoms arrange themselves in these forms. Actually, until now there is no well defined law can account for the crystalline structure of materials. Here we show that the crystalline accommodation law, which is theoretically derived and experimentally verified, can explain the crystalline structure of all types of phases. This law is derived directly from the quantum conditions on the free electrons Fermi gas inside the crystal. The new law relates both the volume of Fermi sphere V_F and volume of Brillouin zone V_B to the valence electron concentration VEC as, $\frac{V_F}{V_B} = n \frac{VEC}{2}$ for all crystalline systems and phases, where n is the number of atoms per lattice point or primitive cell. Also because of this law, we introduce the occupied electronic quantum states notation (OEQS), which determine the number of occupied zones in the valence band.

Indexing terms/Keywords

Fermi sphere, Brillouin zone, Valence electron concentration, Crystal Systems, Primitive Cell, Hume-Rothery rules, crystalline accommodation law, OEQS notation.

Academic Discipline And Sub-Disciplines

Physics, Materials Physics.

SUBJECT CLASSIFICATION

Crystal Structure.

TYPE (METHOD/APPROACH)

Theoretical, Experimental and Calculations.

INTRODUCTION

All crystalline materials crystallize in one of seven crystalline systems which have different shapes and sizes. Why crystalline materials take particular forms of crystals and what make the atoms arrange themselves in these forms. Actually, until now there is no well defined law can account for the crystalline structure of materials. The first attempt to answer this question was initiated by Hume Rothery rules and his coworkers [1] formulated in 1926. These rules include solid solubility rules and electron concentration rule. Solubility rules account for the solid solubility in alloys and include; the atomic size factor, the electrochemical effect and the relative valency effect. Electron concentration rule states that at particular value of valence electron concentration ratio (VEC), intermetallic compounds are formed and have the same crystal structure. These compounds are termed electron compounds or Hume-Rothery compounds and do not obey the valency laws of chemistry. They are divided into three categories according to the value of VEC as the following; $VEC = 3/2$ β -brass (bcc), $VEC = 21/13$ γ -brass (complex cubic) and $VEC = 7/4$ ϵ -brass (cph).

The intermediate phases, which formed in alloys, are of three types; electrochemical compounds, electron compounds and size-factor compounds. Electrochemical compounds obey the valency laws of chemistry and are formed when one element is electropositive and the other is electronegative. Size-factor compounds are formed when the difference in atomic diameter is appreciable. Hume-Rothery electron concentration rule accounts only for the electron compounds not for electrochemical or size-factor compounds. In 1936, Mott and Jones [2] could successfully interpret the Hume-Rothery electron concentration rule in terms of the contact of the Fermi sphere with the set of Brillouin zone planes specific to a given phase. This has come to be known as the Fermi surface-Brillouin zone interaction, FsBz. They proposed that the stability of given phase is enhanced, when the Fermi sphere touches the relevant Brillouin zone planes, leading to the so-called matching condition or interference condition $2k_F = |\mathbf{G}|$, where $2k_F$ is the Fermi sphere diameter and $|\mathbf{G}|$ is the magnitude of the reciprocal lattice vector corresponding to the relevant Brillouin zone planes. Mizutani and coworkers [3-12] have developed a technique to extract the FsBz interaction based on first-principle FLAPW (full potential linearized augmented plane wave) electronic structure calculations. The FLAPW were performed for the Ag_5Li_8 gamma brass and it is found that the Hume-Rothery stabilization mechanism fails for this compound and proposed a new stability mechanism, in which the unique gamma brass structure can effectively lower the band-structure energy by forming heavily populated bonding states near the bottom of Ag-4d band [7]. In addition, the FLAPW- Fourier analysis led to formulation of new Hume-Rothery electron concentration rule [13] based on the interference condition. The new rule can cover a wider



range of alloys than the empirical Hume-Rothery rule, which was validated only for noble metal alloys. Actually, the new rule also cannot account for all crystalline phases. The failure of Hume Rothery rule and the new rule comes from including $|G|$ into the rule, because $|G|$ is not fixed for any given structure and varies with the direction.

The term accommodation law is first introduced in this paper. It originates from the work of Tarek El Ashram [14,15] as a new condition for crystalline phase formation and stability. Crystalline accommodation here means the capability of a crystal to adapt its structure to accommodate the valence electrons in the allowed quantum electronic states i.e. obey the accommodation law. This law is derived directly from the quantum conditions on the free electrons Fermi gas inside the crystal and it is not an assumption [15]. The crystalline accommodation law relates the volume of Fermi sphere V_F and the volume of Brillouin zone V_B to the valence electron concentration ratio VEC as; $\frac{V_F}{V_B} = n \frac{VEC}{2}$. Where n is the number of atoms per lattice point or primitive cell and VEC ratio is defined as; *the number of the outermost interactive electrons shared in bonding divided by the number of the interacting atoms*. The left hand side of this law can be determined experimentally since V_F is given by, $V_F = \frac{4}{3} \pi k_F^3$ and k_F is the Fermi electron wave vector and can be calculated from Fermi energy as, $E_F = \frac{\hbar^2 k_F^2}{2m}$, which can be measured experimentally. In addition, k_F can be calculated theoretically from the electron concentration as; $k_F = \left(\frac{3\pi^2 N}{V}\right)^{\frac{1}{3}}$, here N/V is the number of valence electrons per unit volume. The volume of Brillouin zone V_B is given by; $V_B = \frac{8\pi^3}{V_p}$, here V_p is the volume of the primitive cell, which can be determined experimentally from the XRD data. The right hand side of the law is calculated theoretically from the number of atoms per lattice point n and the valence electron concentration ratio VEC . Therefore, we aim to verify experimentally the crystalline accommodation law and confirm its validity in explaining the crystalline structure for pure elements and different types of compounds.

2. CALCULATION

2.1 EXPERIMENTAL VERIFICATION OF CRYSTALLINE ACCOMMODATION LAW

The experimental XRD data is obtained from [16] and the experimental data for E_F is obtained from [17]. For Cu (Cubic, $Fm\bar{3}m$) the volume of primitive cell is given by; $V_P = a^3/4$, $a = 3.615 \text{ \AA}$, this gives for $V_P = 11.8104 \text{ \AA}^3$ and for $V_B = 21.0026 \text{ \AA}^3$. $E_F = 6.81 \text{ eV}$, this gives for $k_F = 1.3369 \text{ \AA}^{-1}$ from which $V_F = 10.0088 \text{ \AA}^3$, therefore $V_F/V_B = 0.50037$. Now let us calculate $nVEC/2$, for Cu we have only one atom per lattice point $n=1$ and $VEC = 1$, therefore $nVEC/2 = 0.5$ which is in a good agreement with the experimental calculated value for V_F/V_B . By the same method of calculation, we get the same result for Gold (Au), silver (Ag) and Aluminum (Al) elements (see Table 1).

Table 1. Experimental verification of crystalline accommodation law.

Element	VEC	System S.G.	n	E_F (th) eV	E_F (ex) eV	V_B \AA^3	V_F \AA^3	V_F/V_B	$nVEC/2$	Diff.
Au	1	Cubic $Fm\bar{3}m$	1	5.52	5.57	14.6132	7.4039	0.5066	0.5	0.0066
Ag	1	Cubic $Fm\bar{3}m$	1	5.48	5.23	14.550	6.7367	0.4630	0.5	0.0370
Cu	1	Cubic $Fm\bar{3}m$	1	7.04	6.81	21.0026	10.0088	0.50037	0.5	0.00037
Zn	2	Hexagonal $P6_3/mmc$	2	9.39	9.44	8.1521	16.3343	2.0036	2.0	0.0036
Al	3	Cubic $Fm\bar{3}m$	1	11.66	11.65	14.9401	22.3970	1.4991	1.5	0.0009
Sn	4	Tetragonal $I4_1/amd$	2	9.99	9.82	4.5854	17.3315	3.7797	4.0	0.2203

For Zn (Hexagonal, $P6_3/mmc$) the volume of primitive cell is given by; $V_P = a^2 c \sqrt{3}/2$, $a = 2.665 \text{ \AA}$ $c = 4.947$ this gives for $V_P = 30.4275 \text{ \AA}^3$ and for $V_B = 8.1521 \text{ \AA}^3$. $E_F = 9.44 \text{ eV}$ this gives for $k_F = 1.5740 \text{ \AA}^{-1}$ from which $V_F = 16.3343 \text{ \AA}^3$, therefore $V_F/V_B = 2.0036$. Now let us calculate $nVEC/2$ for Zn, we have two atoms per lattice point $n=2$ and $VEC = 2$, therefore $nVEC/2 = 2$ which is in a good agreement with the experimental calculated value for V_F/V_B . (see Table 1). For β -Sn (Tetragonal, $I4_1/amd$) the volume of primitive cell is given by; $V_P = a^2 c/2$, $a = 5.831 \text{ \AA}$ $c = 3.182$ this gives for $V_P = 54.0948 \text{ \AA}^3$ and for $V_B = 4.5854 \text{ \AA}^3$. $E_F = 9.82 \text{ eV}$ this gives for $k_F = 1.6054 \text{ \AA}^{-1}$ from which $V_F = 17.3315 \text{ \AA}^3$, therefore $V_F/V_B = 3.7797$. Now let us calculate $nVEC/2$ for β -Sn, we have two atoms per lattice point $n=2$ and $VEC = 4$, therefore $nVEC/2 = 4$ which is in a good agreement with the experimental calculated value for V_F/V_B . (see Table 1).



2.2 THE VALIDITY OF CRYSTALLINE ACCOMMODATION LAW FOR INTERMEDIATE AND COMPLEX PHASES

Actually, there is no experimental data available for E_F for intermetallic compounds, however we can see from Table 1 that the experimental and theoretical values of E_F are nearly the same. Therefore we will determine the value of E_F theoretically.

2.2.1 Electrochemical Compounds

For NaCl (Cubic, $Fm\bar{3}m$) the volume of primitive cell is given by: $V_P = a^3/4$, $a = 5.642 \text{ \AA}$ this gives for $V_P = 44.8992 \text{ \AA}^3$ and for $V_B = 21.0026 \text{ \AA}^3$. $E_F = 11.546 \text{ eV}$ this gives for $k_F = 1.7408 \text{ \AA}^{-1}$ from which $V_F = 22.0984 \text{ \AA}^3$, therefore $V_F/V_B = 4.000073$. Now let us calculate $nVEC/2$ for NaCl, we have two atoms per lattice point $n=2$ and $VEC = (1 \times 1 + 1 \times 7)/2 = 4$, therefore $nVEC/2 = 4$ which is in a good agreement with the experimental calculated value for V_F/V_B (see Table 2).

Table 2. The validity of crystalline accommodation law for different types of compounds.

Compound	VEC	System S.G.	n	E_F (eV)	V_B (\AA^3)	V_F (\AA^3)	V_F/V_B	$nVEC/2$	Diff.
1. Electrochemical Compounds									
NaCl	4	Cubic $Fm\bar{3}m$	2	11.546	5.5245	22.0984	4.000073	4	.00007
Mg ₂ Sn	8/3	Cubic $Fm\bar{3}m$	3	8.045	3.2133	12.8532	4.000012	4	.00001
Mg ₂ Pb	8/3	Cubic $Fm\bar{3}m$	3	7.918	3.1375	12.550	4.00000	4	0
CaF ₂	16/3	Cubic $Fm\bar{3}m$	3	19.549	6.0856	48.6851	8.000056	8	.00005
2. Size-factor Compounds									
MgCu ₂	4/3	Cubic $Fd\bar{3}m$	6	7.428	2.8509	11.4038	4.0001	4	.0001
AgBe ₂	5/3	Cubic $Fd\bar{3}m$	6	10.745	3.9680	19.8403	5.000076	5	.00007
Au ₂ Bi	7/3	Cubic $Fd\bar{3}m$	6	8.427	1.9687	13.7811	7.00013	7	.00013
BaMg ₂	2	Hexagonal $P6_3/mmc$	12	5.511	0.6073	7.2881	12.00083	12	.00083
MgZn ₂	2	Hexagonal $P6_3/mmc$	12	8.779	1.221	14.6524	12.00038	12	.00038
3. Electron Compounds									
CuZn	3/2	Cubic $Pm\bar{3}m$	2	8.727	9.6818	14.5227	1.50000	1.5	0
CuBe	3/2	Cubic $Pm\bar{3}m$	2	10.381	12.5603	18.8405	1.500011	1.5	.00011
AgCd	3/2	Cubic $Pm\bar{3}m$	2	6.832	6.7066	10.0599	1.500003	1.5	.00003
Cu ₅ Zn ₈	21/1 3	Cubic $I\bar{4}3m$	26	8.873	0.7089	14.8882	21.0018	21	.0018
Cu ₉ Al ₄	21/1 3	Cubic $P\bar{4}3m$	52	9.234	0.3763	15.8061	42.0041	42	.0041
Ag ₅ Cd ₈	21/1 3	Cubic $I\bar{4}3m$	26	7.0184	0.4987	10.4729	21.0000	21	0
AgZn ₃	7/4	Hexagonal $P6_3/mmc$	4	13.652	8.1195	28.4145	3.4995	3.5	.0005
AgCd ₃	7/4	Hexagonal $P6_3/mmc$	4	11.530	6.3007	22.0523	3.4999	3.5	.0001
AuCd ₃	7/4	Hexagonal $P6_3/mmc$	24	7.096	0.5070	10.6476	21.0012	21	.0012
Ag ₅ Li ₈	1	Cubic $I\bar{4}3m$	26	5.1763	0.5102	6.6333	13.00013	13	.00001



2.2.2 Size-Factor Compounds

For Au_2Bi (Cubic, $Fd\bar{3}m$) the volume of primitive cell is given by; $V_P = a^3/4$, $a = 7.958 \text{ \AA}$ this gives for $V_P = 125.9945 \text{ \AA}^3$ and for $V_B = 1.9687 \text{ \AA}^3$. $E_F = 8.427 \text{ eV}$ this gives for $k_F = 1.4873 \text{ \AA}^{-1}$ from which $V_F = 13.7811 \text{ \AA}^3$, therefore $V_F/V_B = 7.00013$. Now let us calculate $nVEC/2$ for Au_2Bi , we have six atoms per lattice point $n = 6$ and $VEC = (2 \times 1 + 1 \times 5)/3 = 4$, therefore $nVEC/2 = 7$ which is in a good agreement with the experimental calculated value for V_F/V_B (see Table 2).

2.2.3 Elecron Compounds

For $VEC = 3/2$, let us take $CuZn$ (Cubic, $Pm\bar{3}m$) the volume of primitive cell is given by; $V_P = a^3$, $a = 7.958 \text{ \AA}$ this gives for $V_P = 25.6201 \text{ \AA}^3$ and for $V_B = 9.6818 \text{ \AA}^3$. $E_F = 8.727 \text{ eV}$ this gives for $k_F = 1.5135 \text{ \AA}^{-1}$ from which $V_F = 14.5227 \text{ \AA}^3$, therefore $V_F/V_B = 1.500009$. Now let us calculate $nVEC/2$ for $CuZn$, we have 2 atoms per lattice point $n = 2$ and $VEC = (1 \times 1 + 1 \times 2)/2 = 3/2$, therefore $nVEC/2 = 1.5$ which is in a good agreement with the experimental calculated value for V_F/V_B (see Table 2). For $VEC = 21/13$, let us take Cu_9Al_4 (Cubic, $P\bar{4}3m$) the volume of primitive cell is given by; $V_P = a^3$, $a = 8.7027 \text{ \AA}$ this gives for $V_P = 659.1162 \text{ \AA}^3$ and for $V_B = 0.3763 \text{ \AA}^3$. $E_F = 9.2345 \text{ eV}$ this gives for $k_F = 1.5568 \text{ \AA}^{-1}$ from which $V_F = 15.8061 \text{ \AA}^3$, therefore $V_F/V_B = 42.0041$. Now let us calculate $nVEC/2$ for Cu_9Al_4 , we have 52 atoms per lattice point $n = 52$ and $VEC = (9 \times 1 + 4 \times 3)/13 = 21/13$, therefore $nVEC/2 = 42$ which is in a good agreement with the experimental calculated value for V_F/V_B (see Table 2). For $VEC = 7/4$, let us take $AgZn_3$ (Hexagonal, $P6_3/mmc$) the volume of primitive cell is given by; $V_P = a^2 c \sqrt{3}/2$, $a = 2.8227 \text{ \AA}$, $c = 4.4274 \text{ \AA}$ this gives for $V_P = 30.5498 \text{ \AA}^3$ and for $V_B = 8.1195 \text{ \AA}^3$. $E_F = 13.65 \text{ eV}$ this gives for $k_F = 1.8930 \text{ \AA}^{-1}$ from which $V_F = 28.4183 \text{ \AA}^3$, therefore $V_F/V_B = 3.4995$. Now let us calculate $nVEC/2$ for $AgZn_3$, we have 4 atoms per lattice point $n = 4$ and $VEC = (1 \times 1 + 3 \times 2)/4 = 7/4$, therefore $nVEC/2 = 3.5$, which is in a good agreement with the experimental calculated value for V_F/V_B (see Table 2). For complex phase Ag_5Li_8 (Cubic, $I\bar{4}3m$) the volume of primitive cell is given by; $V_P = a^3/2$, $a = 9.9066 \text{ \AA}$ this gives for $V_P = 486.1204 \text{ \AA}^3$ and for $V_B = 0.5102 \text{ \AA}^3$. $E_F = 5.1763 \text{ eV}$ this gives for $k_F = 1.1656 \text{ \AA}^{-1}$ from which $V_F = 6.6333 \text{ \AA}^3$, therefore $V_F/V_B = 13.00013$. Now let us calculate $nVEC/2$ for Ag_5Li_8 , we have 26 atoms per lattice point $n = 26$ and $VEC = (5 \times 1 + 8 \times 1)/13 = 13/13 = 1$, therefore $nVEC/2 = 13$, which is in a good agreement with the experimental calculated value for V_F/V_B (see Table 2).

3. RESULTS AND DISSCUSION

It is clear from Table 1 that the experimental $(\frac{V_F}{V_B})$ and theoretical $(n \frac{VEC}{2})$ values are very consistent. This is a conclusive evidence on the validity of crystalline accommodation law. The success of this law comes from including V_B , which is fixed for any given structure instead of $|G|$ which is not fixed and varies with the direction, into the law. Here we can not account for all elements and compounds but actually, this law can explain any crystal structure. A very important note is that this law gives the number of occupied electronic quantum states (OEQS). This number as we see from Table 1 is either integer or half integer which indicates that the state may be filled or half filled. Every Brillouin zone accommodates only one state and every state accommodates only two electrons of opposite spins, if it is filled, or one electron, if it is half filled. This also indicates the validity of this law, for example let us take Cu; $\frac{V_F}{V_B} = n \frac{VEC}{2} = 0.5$ this means for Cu we have only the first zone half filled. Let us represent the number of occupied electronic quantum state notation (OEQS) for Cu as $1Bz^{0.5}$. By the same way we can represent the OEQS for Zn as $2Bz$ (two filled zones), Al as $2Bz^{0.5}$ (two zones, the first is filled and the second is half filled) and Sn as $4Bz$ (four filled zones, see Table 3).

Table 3. The OEQS for some elements

Element	VEC	System S.G.	n	nVEC/2	OEQS
Au	1	Cubic $Fm\bar{3}m$	1	0.5	$1Bz^{0.5}$
Ag	1	Cubic $Fm\bar{3}m$	1	0.5	$1Bz^{0.5}$
Cu	1	Cubic $Fm\bar{3}m$	1	0.5	$1Bz^{0.5}$
Zn	2	Hexagonal $P6_3/mmc$	2	2.0	$2Bz$
Al	3	Cubic $Fm\bar{3}m$	1	1.5	$2Bz^{0.5}$
Sn	4	Tetragonal $I4_1/amd$	2	4.0	$4Bz$

For compounds, it is clear from Table 2 that the experimental $(\frac{V_F}{V_B})$ and theoretical $(n \frac{VEC}{2})$ values are very consistent. Therefore the crystal accommodation law can explain the crystalline structure for different types of compounds including



complex structures. The OEQS for these compounds are represented in Table 4. For example the OEQS for Cu_9Al_4 is 42Bz (42 filled zones), these zones are overlapped, because there is no gaps in the valence band.

Table 4. The OEQS for some compounds.

Compound	VEC	System S.G.	n	nVEC/2	OEQS
NaCl	4	Cubic $\text{Fm}\bar{3}\text{m}$	2	4	4Bz
Mg_2Sn	8/3	Cubic $\text{Fm}\bar{3}\text{m}$	3	4	4Bz
Mg_2Pb	8/3	Cubic $\text{Fm}\bar{3}\text{m}$	3	4	4Bz
CaF_2	16/3	Cubic $\text{Fm}\bar{3}\text{m}$	3	8	8Bz
MgCu_2	4/3	Cubic $\text{Fd}\bar{3}\text{m}$	6	4	4Bz
AgBe_2	5/3	Cubic $\text{Fd}\bar{3}\text{m}$	6	5	5Bz
Au_2Bi	7/3	Cubic $\text{Fd}\bar{3}\text{m}$	6	7	7Bz
BaMg_2	2	Hexagonal $\text{P6}_3/\text{mmc}$	12	12	12Bz
MgZn_2	2	Hexagonal $\text{P6}_3/\text{mmc}$	12	12	12Bz
CuZn	3/2	Cubic $\text{Pm}\bar{3}\text{m}$	2	1.5	$2\text{Bz}^{0.5}$
CuBe	3/2	Cubic $\text{Pm}\bar{3}\text{m}$	2	1.5	$2\text{Bz}^{0.5}$
AgCd	3/2	Cubic $\text{Pm}\bar{3}\text{m}$	2	1.5	$2\text{Bz}^{0.5}$
Cu_5Zn_8	21/13	Cubic $\text{I}\bar{4}3\text{m}$	26	21	21Bz
Cu_9Al_4	21/13	Cubic $\text{P}\bar{4}3\text{m}$	52	42	42Bz
Ag_5Cd_8	21/13	Cubic $\text{I}\bar{4}3\text{m}$	26	21	21Bz
AgZn_3	7/4	Hexagonal $\text{P6}_3/\text{mmc}$	4	3.5	$4\text{Bz}^{0.5}$
AgCd_3	7/4	Hexagonal $\text{P6}_3/\text{mmc}$	4	3.5	$4\text{Bz}^{0.5}$
AuCd_3	7/4	Hexagonal $\text{P6}_3/\text{mmc}$	24	21	21Bz
Ag_5Li_8	1	Cubic $\text{I}\bar{4}3\text{m}$	26	13	13Bz

4. CONCLUSION

In conclusion, the crystalline accommodation law, $\frac{V_F}{V_B} = n \frac{VEC}{2}$, which is theoretically derived and experimentally verified, can successfully account for the crystalline structure of all types of crystalline phases. According to this law, the crystal adapts its structure in such a way to accommodate the valence electrons into the allowed electronic quantum states. Because of this law, we introduce the occupied electronic states notation (OEQS) for different types of crystalline phases to account for the number of filled zones in the valence band.



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