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Three kinds of Electrons in Metal Crystals. Band theory of a Metal from the side of its Crystal Lattice

Henadzi Filipenka

Independent researcher, Researcher at Institute of Modern Knowledge Minsk, Belarus

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Abstract

The literature generally describes a metallic bond as the one formed by means of mutual bonds between atoms' exterior electrons and not possessing the directional properties. However, attempts have been made to explain directional metallic bonds, as a specific crystal metallic lattice.

This paper demonstrates that the metallic bond in the densest packings (volume-centered and face- centered) between the centrally elected atom and its neighbours in general is, probably, effected by 9 (nine) directional bonds, as opposed to the number of neighbours which equals 12 (twelve) (coordination number).

Probably, 3 (three) "foreign" atoms are present in the coordination number 12 stereometrically, and not for the reason of bond. This problem is to be solved experimentally.

***Corresponding author:** Henadzi Filipenka, Independent researcher, Researcher at Institute of Modern Knowledge Minsk, Belarus.

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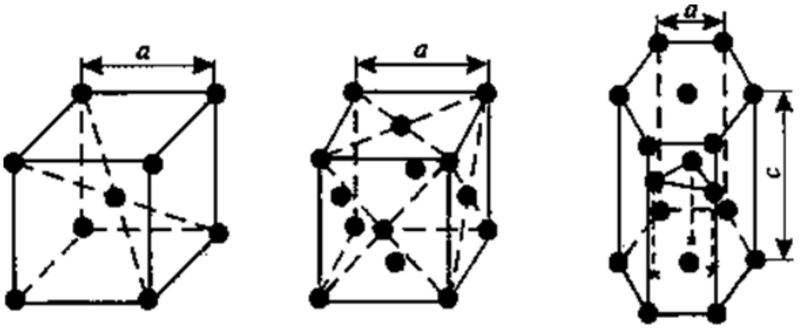
The main problem is that using X-rays, the types of crystal lattices of different metals were determined, and why they are such and not others is not yet known. For example, copper crystallizes in the fcc lattice, and iron in the bcc lattice, which, when heated, becomes fcc and this transition is used in heat treatment of steels.

Usually in the literature, the metallic bond is described as carried out through the socialization of the outer electrons of the atoms and does not possess the property of directionality. Although there are attempts (see below) to explain the directional metal bond since the elements crystallize into a specific type of lattice. The main types of crystal lattices of metals are body centered cubic; face-centered cubic; hexagonal close-packed. It is still impossible in the general case to deduce the crystal structure of a metal from the electronic structure of the atom from quantum-mechanical calculations, although, for example, Ganzhorn and Delinger pointed out a possible connection between the presence of a cubic body-centered lattice in the subgroups of titanium, vanadium, chromium and the presence of valence d-orbitals in the atoms of these metals. It is easy to see that the four hybrid orbitals are directed along the four solid diagonals of the cube and are well suited for connecting each atom with its 8 neighbors in a body-centered cubic lattice. In this case, the remaining orbitals are directed to the centers of the unit cell faces and, possibly, can take part in the bond of the atom with its six second neighbors. The first coordination number (K.CH.1) \ “8 \” plus the second coordination number (K.CH.2) \ “6 \” in total is \ “14 \”. Let us show that the metallic bond in the closest packing (HEC and FCC) between a centrally selected atom and its neighbors, in the general case, is presumably carried out through 9 (nine) directional bonds, in contrast to the number of neighbors equal to 12 (twelve) the first (coordination number) ... The second (K.P. 2 \ ‘’ 6 \ ‘’ in total is \ ‘’ 18 \ ‘’.

In the literature, there are many factors affecting crystallization, so I decided to remove them as much as possible, and the metal model in the article, let’s say, is ideal, i.e. all atoms are the same (pure metal), crystal lattices without inclusions, without interstices, without defects, etc. Using the Hall effect and other data on properties, as well as calculations by Ashcroft and Mermin, for me the main factor determining the type of lattice turned out to be the outer electrons of the core of an atom or ion, which resulted from the transfer of some of the outer electrons to the conduction band. It turned out that the metallic bond is due not only to the socialization of electrons, but also to the outer electrons of the atomic cores, which determine the direction or type of the crystal lattice.



a) б) в)

How did I start to build models of ideal single crystals of pure metals? Ideal crystals for getting away from dependence on lattice defects, impurities and other inclusions. Using simple examples, we will show that one bond for a diamond at a density packing 34% and coordination number 4 account for 34%: 4 = 8.5%. The cubic primitive lattice has a packing density of 52% and coordination number 6 accounts for 52%: 6 = 8.66%. For a cubic body-centered lattice, the packing density is 68% and coordination number 8 accounts for 68%: 8 = 8.5%. For a cubic face-centered lattice, the packing density is 74% and the coordination number 12 is 74%: 12 = 6.16% (!!!), and if 74%: 9 = 8.22%. For a hexagonal lattice, the packing density is 74% and the coordination number 12 is 74%: 12 = 6.16%, and if 74%: 9 = 8.22%. (!!!) Obviously, these 8.66-8.22% carry some physical meaning. The remaining 26% are multiples of 8.66 and 100% hypothetical packing density is possible with 12 bonds. But is such a possibility real? The outer electrons of the last shell or subshells of the metal atom form the conduction band. The number of electrons in the conduction band affects the Hall constant, the compression ratio, etc. Let us construct a model of an element metal so that the remaining, after filling the conduction band, the outer electrons of the last shell or subshells of the atomic core in some way affect the structure of the crystal structure (for example: for the bcc lattice-8 “valence” electrons, and for HEC and FCC -12 or 9). As a result of studying the lattices of chemical elements, we can say that the bcc lattices of light elements are formed by 8 bond electrons, and heavy 14 electrons of the atomic core. FCC lattices are formed by 9 bond electrons for light elements and 15 for heavy ones.

Then I began to fill the conduction band with external electrons. One of the remarkable features of the Hall effect is, however, that in some metals the Hall coefficient is positive, and therefore the carriers in them should apparently have a charge opposite to the charge electron. This property required clarification. Option one: a thin closed tube, completely filled with electrons except one. With such a filling of the zone, with the local movement of an electron, the opposite movement of the \ “place \” of the electron, which has not filled the tube, is observed, that is, the movement of a non-negative charge. Option two: there is one electron in the tube, therefore, only one charge, a negatively charged electron, can move. It can be seen from these two extreme variants that the sign of the carriers determined by the Hall coefficient should, to some extent, depend on the filling of the conduction band with electrons. Let us fill the conduction band with electrons so that the outer electrons of the atomic cores influence on the formation of a type of crystallization lattice. Let us assume that the number of external bond electrons on the last shell of the atomic core, after filling the conduction band, is equal to the number of neighboring atoms (coordination number) in the crystal lattice. It turned out that the metallic bond is due not only to the socialization of electrons, but also to the outer electrons of the atomic cores, which determine the direction or type of the crystal lattice. Let’s try to connect the outer electrons of an atom of a given element with the structure of its crystal lattice, taking into account the need for directed bonds (chemistry) and the presence of socialized electrons (physics) responsible for the galvanomagnetic properties.

Introduction

At present, it is impossible, as a general case, to derive by means of quantum-mechanical calculations the crystalline structure of metal in relation to electronic structure of the atom. However, Hanzhorn and Dellinger indicated a possible relation between the presence of a cubical volume-centered lattice in subgroups of titanium, vanadium, chrome and availabilty in these metals of valent d-orbitals. It is easy to notice that the four hybrid orbitals are directed along the four physical diagonals of the cube and are well adjusted to binding each atom to its eight neighbours in the cubical volume-centered lattice, the remaining orbitals being directed towards the edge centers of the element cell and, possibly, participating in binding the atom to its six second neighbours /3/p. 99.

Let us try to consider relations between exterior electrons of the atom of a given element and structure of its crystal lattice, accounting for the necessity of directional bonds (chemistry) and availability of combined electrons (physics) responsible for galvanic and magnetic properties.

According to /1/p. 20, the number of Z-electrons in the conductivitiy zone has been obtained by the authors, allegedly, on the basis of metal’s valency towards oxygen, hydrogen and is to be subject to doubt, as the experimental data of Hall and the uniform compression modulus are close to the theoretical values only for alkaline metals. The volume-centered lattice, Z=1 casts no doubt. The coordination number equals 8.

The exterior electrons of the final shell or subcoats in metal atoms form conductivity zone. The number of electrons in the conductivity zone effects Hall’s constant, uniform compression ratio, etc.

Let us construct the model of metal - element so that external electrons of last layer or sublayers of atomic kernel, left after filling the conduction band, influenced somehow pattern of crystalline structure (for example: for the body-centred lattice - 8 ‘valency’ electrons, and for volume-centered and face- centred lattices - 12 or 9).

Rough, qualitative measurement of number of electrons in conduction band of metal - element. Explanation of factors, influencing formation of type of monocrystal matrix and sign of hall constant. (Algorithm of construction of model)

The measurements of the Hall field allow us to determine the sign of charge carriers in the conduction band. One of the remarkable features of the Hall effect is, however, that in some metals the Hall coefficient is positive, and thus carriers in them should, probably, have the charge, opposite to the electron charge /1/.

At room temperature this holds true for the following: vanadium, chromium, manganese, iron, cobalt, zinc, circonium, niobium, molybdenum, ruthenium, rhodium, cadmium, cerium, praseodymium, neodymium, ytterbium, hafnium, tantalum, wolfram, rhenium, iridium, thallium, plumbum /2/. Solution to this enigma must be given by complete quantum - mechanical theory of solid body. Roughly speaking, using the base cases of Born-Karman, let us consider a highly simplified case of one- dimensional conduction band. The first variant: a thin closed tube is completely filled with electrons but one. The diameter of the electron roughly equals the diameter of the tube.

With such filling of the area at local movement of the electron an opposite movement of the 'site' of the electron, absent in the tube, is observed, i.e. movement of non-negative sighting. The second variant: there is one electron in the tube - movement of only one charge is possible - that of the electron with a negative charge. These two opposite variants show, that the sighting of carriers, determined according to the Hall coefficient, to some extent, must depend on the filling of the conduction band with electrons. Figure 1.

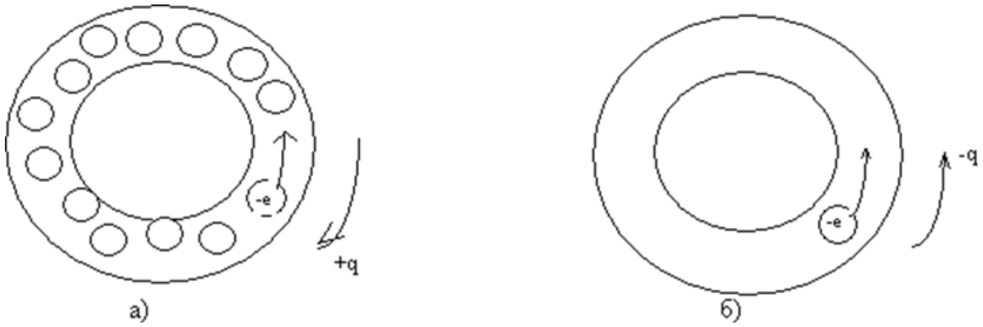


Figure 1: Schematic representation of the conduction band of two different metals. (scale is not observed).

- the first variant;
- the second variant.

The order of electron movement will also be affected by the structure of the conductivity zone, as well as by the temperature, admixtures and defects. Magnetic quasi-particles, magnons, will have an impact on magnetic materials.

Since our reasoning is rough, we will further take into account only filling with electrons of the conductivity zone. Let us fill the conductivity zone with electrons in such a way that the external electrons of the atomic kernel affect the formation of a crystal lattice. Let us assume that after filling the conductivity zone, the number of the external electrons on the last shell of the atomic kernel is equal to the number of the neighbouring atoms (the coordination number) (5).

The coordination number for the volume-centered and face-centered densest packings are 12 and 18, whereas those for the body-centered lattice are 8 and 14 (3).

The below table is filled in compliance with the above judgements.

Element	**R_H . 10^{10} (м^3/K)**	**Z. (number)**	**Z kernel (number)**	**Lattice type**
Na	-2,30	1	8	body-centered
Mg	-0,90	1	9	volume-centered
Al	-0,38	2	9	face-centered
Al	-0,38	1	12	face-centered
K	-4,20	1	8	body-centered
Ca	-1,78	1	9	face-centered
Ca	T=737K	2	8	body-centered
Sc	-0,67	2	9	volume-centered
Sc	-0,67	1	18	volume-centered
Ti	-2,40	1	9	volume-centered
Ti	-2,40	3	9	volume-centered
Ti	T=1158K	4	8	body-centered
V	+0,76	5	8	body-centered
Cr	+3,63	6	8	body-centered
Fe	+8,00	8	8	body-centered
Fe	+8,00	2	14	body-centered
Fe	T=1189K	7	9	face-centered
Fe	T=1189K	4	12	face-centered
Co	+3,60	8	9	volume-centered
Co	+3,60	5	12	volume-centered
Ni	-0,60	1	9	face-centered
Cu	-0,52	1	18	face-centered
Cu	-0,52	2	9	face-centered
Zn	+0,90	2	18	volume-centered
Zn	+0,90	3	9	volume-centered
Rb	-5,90	1	8	body-centered
Y	-1,25	2	9	volume-centered
Zr	+0,21	3	9	volume-centered
Zr	T=1135K	4	8	body-centered
Nb	+0,72	5	8	body-centered
Mo	+1,91	6	8	body-centered
Ru	22	7	9	volume-centered
Rh	+0,48	5	12	face-centered
Rh	+0,48	8	9	face-centered
Pd	-6,80	1	9	face-centered
Ag	-0,90	1	18	face-centered
Ag	-0,90	2	9	face-centered
Cd	+0,67	2	18	volume-centered
Cd	+0,67	3	9	volume-centered
Cs	-7,80	1	8	body-centered
La	-0,80	2	9	volume-centered

Ce	+1,92	3	9	face-centered
Ce	+1,92	1	9	face-centered
Pr	+0,71	4	9	volume-centered
Pr	+0,71	1	9	volume-centered
Nd	+0,97	5	9	volume-centered
Nd	+0,97	1	9	volume-centered
Gd	-0,95	2	9	volume-centered
Gd	T=1533K	3	8	body-centered
Tb	-4,30	1	9	volume-centered
Tb	T=1560K	2	8	body-centered
Dy	-2,70	1	9	volume-centered
Dy	T=1657K	2	8	body-centered
Er	-0,341	1	9	volume-centered
Tu	-1,80	1	9	volume-centered
Yb	+3,77	3	9	face-centered
Yb	+3,77	1	9	face-centered
Lu	-0,535	2	9	volume-centered
Hf	+0,43	3	9	volume-centered
Hf	T=2050K	4	8	body-centered
Ta	+0,98	5	8	body-centered
W	+0,856	6	8	body-centered
Re	+3,15	6	9	volume-centered
Os	<0	4	12	volume-centered
Ir	+3,18	5	12	face-centered
Pt	-0,194	1	9	face-centered
Au	-0,69	1	18	face-centered
Au	-0,69	2	9	face-centered
Tl	+0,24	3	18	volume-centered
Tl	+0,24	4	9	volume-centered
Pb	+0,09	4	18	face-centered
Pb	+0,09	5	9	face-centered

Where Rh is the Hall's constant (Hall's coefficient) Z is an assumed number of electrons released by one atom to the conductivity zone. Z kernel is the number of external electrons of the atomic kernel on the last shell. The lattice type is the type of the metal crystal structure at room temperature and, in some cases, at phase transition temperatures (1).

Conclusions

In spite of the rough reasoning the table shows that the greater number of electrons gives the atom of the element to the conductivity zone, the more positive is the Hall's constant. On the contrary the Hall's constant is negative for the elements which have released one or two electrons to the conductivity zone, which doesn't contradict to the conclusions of Payerls. A relationship is also seen between the conductivity electrons (Z) and valency electrons (Z kernel) stipulating the crystal structure.

The phase transition of the element from one lattice to another can be explained by the transfer of one of the external electrons of the atomic kernel to the metal conductivity zone or its return from the conductivity zone to the external shell of the kernel under the influence of external factors (pressure, temperature).

We tried to unravel the puzzle, but instead we received a new puzzle which provides a good explanation for the physico-chemical properties of the elements. This is the "coordination number" 9 (nine) for the face-centered and volume-centered lattices.

This frequent occurrence of the number 9 in the table suggests that the densest packings have been studied insufficiently.

Using the method of inverse reading from experimental values for the uniform compression towards the theoretical calculations and the formulae of Arkshoft and Mermin (1) to determine the Z value, we can verify its good agreement with the data listed in Table 1.

The metallic bond seems to be due to both socialized electrons and "valency" ones - the electrons of the atomic kernel.

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