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Extended and in-depth theory of metallic bonds

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Introduction

The main problem is that, using X-rays, the types of crystal lattices of different metals were determined, and why they are so 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 have 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 in the atoms of these metals -orbitals. 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 bonding 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 (C.Ch.2) \ "6 \" in total is \ "14 \".

Discussion

Let us show that the metallic bond in the closest packing (HEC and FCC) between the 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) (coordination number).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 electrons to the conduction band.

Conclusion

It turned out that the metallic bond is due not only to the sharing 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 galvanomagnetic properties.

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