

# The Structure of Metals and its Influence on Metallic Properties

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## Abstract

This article briefly reviews the current model of metallic structure. An alternative model of metallic structure is described. Limitations of the “ions in a sea of electrons/delocalized electrons” model are provided and properties of metals which can be accounted for by the alternative soft-sphere model are discussed. Data from this alternative proposed model that are used to calculate densities, lattice energies, work functions, and internuclear distances are shown to give good agreement with observed values.

**Keywords:** Metallic structure; Densities of metals; Metallic radii; Band theory; Enthalpy of formation; Work function; Catalysis; Free electrons in metals

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## Introduction

The majority of elements that naturally occur on earth are metals. With the exception of mercury, all metals are solids at room temperature and atmospheric pressure. Metals are good conductors of heat and electricity and most metals have high densities and are malleable and ductile. Some transition metals are also known to be good heterogeneous catalysts. Although it is known that most metals have hexagonal, cubic close packed or body centered cubic structures, metallic structure and properties are not fully understood.

### The model of metallic structure

Paul Drude [1] was the first to propose the “free electron” model for electricity conduction in metals. He proposed that in crystalline metals, positive ions were surrounded by an “electron gas”. Estimates of the number of “free” electrons in a metal have also been suggested [2]. Currently, metallic structure and bonding is still described in some university texts as “bonding which involves the delocalization of electrons throughout the metal solid” [3] or as “metal ions in a sea of electrons” [4]. There are discrepancies between the “free electron” model and the principles/calculations in physics [5]. Recent work [6,7] have also shown that the description of metals as “ions in a sea of electrons” is inadequate. It is sometimes thought that metals are malleable and ductile due to the defects in the solid state. However, defects in the solid state also occur in non-metallic solids such as sulphur and phosphorus and these solids do not show qualities similar to metals. The argument that metals are malleable because one

layer of metal atoms can easily slide over another is also not completely logical because if one layer simply slides over another (in a metal wire for example) then that creates a kink (in the wire) and not a smooth bend and some metals are much harder and malleable than others. There are also other properties (such as the Hall effect [8] and work functions of metals) that cannot be accounted for by the popular “ions in a sea of electrons” or “free” electron model.

### Sources of data

The structures, unit cell constants and internuclear separations of most of the elements in the solid state are provided in The Structures of the Elements [9]. A comprehensive set of observed data of structure and unit cell dimensions in the solid state can also be found in Crystal Data Determinative Tables [10] volumes Two and Four which contain data on metals and inorganic compounds. Structural Inorganic Chemistry [11] also contains reliable structural data with references to original work, including detailed discussions. The Journal Physical and Chemical Reference Data [12] also has structural data and unit cell dimensions of compounds at normal temperature/pressure as well as at elevated temperatures and pressures. The CRC Handbook of Chemistry and Physics [13] contains extensive compilations of many properties of metals including densities, work functions,

relative atomic masses and enthalpies of formation. Observed values of densities, lattice energies, and enthalpies of formation, work functions, unit cell constants and internuclear distances/bond lengths used in this work are quoted from the above publications. Values of unit cell constants/internuclear distances provided by the above publications are often given to at least two and often three or four decimal places of an Angstrom (Å). We have examined many of the unit cell dimensions and internuclear distance listed in these publications and found that usually they agree well and in general if there are differences (in unit cell constants) they are less than 0.01 Å. There is no reason to doubt the reliability of the values in these publications.

### The new alternative model of metallic structure

This alternative model considers atoms and ions as “soft” compressible spheres. It was developed to calculate internuclear distances of ionic and covalent compounds [14,15]. Calculated values when compared with experimental figures produced excellent agreement with average difference between observed and calculated at less than 5% (and for Group 1 and Group 2 binary salts to less than 0.5%). The concept was then extended initially to crystals of Group 1 and Group 2 metals [16] and revised to include transition metals. We consider that in a metal solid, the outermost electron(s) in each atom is/are not exactly “free” nor completely delocalized. The outermost electron(s) is/are separated/detached from the atom which forms a positive ion with one or more of the “detached” electron(s) behaving like negative ions. The detached outermost electron(s) can occupy certain equivalent positions that are at the midpoint between the nearest neighbors of the positive ions (similar to ionic crystals, where positive ions occupy positions between negative ions) but can move within these midpoint positions in a unit cell. For the remainder of this paper, these midpoint positions will be called “midpoint sites”. Depending on the Group and metallic structure (hcp, ccp or bcc) the most likely number of outermost electrons detached from each individual metal atom range from one to a maximum of five. The soft-sphere ionic radii of Group 1 and Group 2 metals (except beryllium) have already been determined very accurately [14] and in this work we use some of these results as examples for the soft-sphere model of metallic structure and bonding. In a crystal with a hexagonal (hcp) or cubic closed pack (ccp) structure of identical atoms, each atom has twelve coordination or twelve closest neighbors and in a body centered cubic each atom has eight closest neighbors. There are two atoms in each unit cell in a body centered cubic, six atoms in each unit in a hexagonal closed pack and four atoms per unit cell in a cubic closed packed or face centered cubic [17] crystal. At room temperature, all Group 1 metals have a bcc structure and each atom has one outermost electron. In the new model, each atom has a single outermost electron which it loses to form a unipositive ( $1^+$ ) ion. Each positive ion has eight nearest identical neighbors of positive ions. Hence there are eight equivalent sites that are midpoint between the internuclear distance of a positive ion and its eight neighboring positive ions. The outermost electron which is detached from the atom can occupy and move around any one of these eight midpoint sites in a unit cell at any one time. Since there are two positive ions in each unit cell, there are only two detached electrons in each cell and, therefore, at any one

time only two of the eight midpoint sites are occupied and the rest are vacant and under certain conditions can be occupied by other detached electrons from other unit cells. Group 2 metals are different. Beryllium and magnesium have hcp structures at room temperature whereas both calcium and strontium possess the ccp structure and barium has a bcc structure respectively [18]. In any Group 2 metal crystal, each metal atom loses its two outermost electrons to form a dipositive ( $2^+$ ) ion. In a barium crystal which has a bcc structure, each dipositive ion has eight identical nearest neighbors of positive ions. Since there are two positive ions in each unit cell, there are four detached electrons in a cell. Hence, at any one time there are four electrons occupying the eight equivalent midpoint sites between the positive ions, which mean that only half of the eight sites are occupied. In calcium and strontium, both with ccp structures, there are four positive ions and eight detached electrons, (with each atom losing two electrons, occupying twenty four equivalent midpoint sites per unit cell. Thus, at any one time, only a third of the sites are occupied. Similarly for beryllium and magnesium, with two positive ions and four detached electrons per cell, at any one time only a third of the twelve sites are occupied. The atomic/metallic radius of a metal atom, which is half the internuclear distance between the nearest neighbors, or distance between the centers of the positive ion and the detached outermost electron, just as in the case of an ionic crystal, can be calculated from the relationship [19]

$$D(\text{calc})^k = [M]^{k+} [e]^{-k} \quad (1)$$

De Broglie proposed that the same dualism of wave and corpuscle as is present in light may also occur in matter [20], where the wavelength of a particle  $\lambda = h/mv$ ,  $h$  being Planck's constant,  $m$  is the mass of the particle and  $v$  its velocity. For a particle moving in an orbit, it was also proposed that  $n\lambda = 2\pi r$ , where  $r$  is the radius of the orbit. According to the de Broglie relationship the electron wave length is directly proportional to its speed and classical physics shows that the speed  $v$  is a function of the coulombic attraction and distance from the nucleus. By making appropriate estimates [21] of screening constants the coulombic attraction and hence approximate values of  $v$  can be obtained. Since the “detached” electron/s in the mid-point sites are attracted equally by two positive ions and we assume that each one moves in orbital motion or radius  $r$  (equal to  $[e]$ ) around the site. Hence, in equation 1,  $D$  is the radius of the metal atom,  $[M]$  is the ionic radius of the positive ion,  $[e]$  is the “orbital radius” of the midpoint site containing the detached electron and the exponent  $k$  is defined in previous work. The value of  $k$  is 1.4, the values of  $[e]$  are 0.41, 0.33, and 0.23 respectively for hcp, bcc and ccp structures. Full details of the rationale and theory of the model are discussed [19] elsewhere and not repeated here. The observed metallic radii (or half the internuclear distance) of Group 1 and Group 2 metals are shown in Column 2 and the radii calculated using previously determined soft-sphere ionic radii and equation 1 are given Column 3 of Table 1 respectively. As shown in Column 4 of the table, differences between the observed and calculated are in all cases less than 0.01 Å. This is very good agreement since the experimental uncertainties of the appropriate cell constants can be as great as 0.01 Å (as in the case of calcium).

**Table 1** Comparison of observed and calculated atomic/metallic radii of Groups 1 Group 2 metals.

Element	Observed (Å)	Soft-sphere calculated (Å)	Obs – Calc (Å)
Li	1.52	1.512	0.008
Na	1.858	1.865	-0.007
K	2.304	2.298	0.006
Rb	2.469	2.474	-0.005
Cs	2.674	2.669	0.005
Be	1.128	1.124	0.004
Mg	1.602	1.61	-0.008
Ca	1.973	1.964	0.009
Sr	2.152	2.158	-0.006
Ba	2.175	2.175	0

### Work function of metals

In the new model of metallic structure, unlike the current “ions in an electron sea” model, the detached outermost electrons can only occupy midpoint sites between two positive ions inside a unit cell, which means that there is almost no detached outermost electron(s) on the surface of the metal. Hence, energy has to be expended to draw those electrons onto the surface of the metal. The work function is an inverse function of the soft-sphere radius since the further the outermost electron(s) is/are from the nucleus of the positive metal ion the less energy is required to draw it/them to the surface. The work functions of metals can be approximated by the following formula:

$$Wk = C_w / [(R)^{1/2}] \quad (2)$$

$Wk$  is the work function,  $R$  is the soft-sphere ionic radius and the constant  $C_w$  has values of 4.75, 5.05 and 5.4 for metals with bcc, hcp and ccp structure respectively. Some examples of results calculated by (2) are shown in Table 2. Column 2 of Table 2 lists the type of structure, Column 3 shows the calculated work functions (in eV) Column 4 shows the observed work functions in eV and the absolute percentage differences are shown in Column 5. The table shows that with the exception of mercury, which is a liquid at room temperature and not a solid, all values agree to better than 90%.

### Enthalpy of formation of metals

We have developed a simple expression to calculate lattice energies of Group 1 and Group 2 salts [14]. The results produced agreed well with lattice energies calculated from the Born-Haber cycle. The expression is as follows:

$$(\text{Lattice energy}) E_L = R(H_o/M)(M^{k-1})/(X^{k-1.3333})(\frac{1}{2}^{0.33333})(\Sigma Q_i^2) \quad (3)$$

where  $R$  is the Rydberg constant for infinite mass converted to kilo Joules per mole,  $H_o$  is the classical Bohr radius,  $M$  is the size of the cation,  $X$  is the size of the anion and  $Q_i$  is the charge on the ions. For example, for sodium chloride  $\Sigma Q_i^2 = 1+1=2$  and for calcium chloride it is  $4+1+1=6$  etc.  $\Sigma Q_i^2$  is the sum of all the squares of the charges on the ions, since the higher the charge on the ions the more electrons need to be removed from the

overlap region and the more energy is required to separate them.  $R$  is the amount of energy needed to remove an electron from a species the size of a hydrogen atom,  $(H_o/M)$  provides a ratio of the distance of the electron from the nucleus, since the greater the size the less is the energy needed to remove the electron.  $(M^{k-1})/(X^{k-1.3333})$  gives an approximation of the overlap, this is multiplied by a factor which is approximated to  $(\frac{1}{2}^{0.33333})$  because the electron is not removed to infinity away from both ions (but rather removed from the overlap region). The expression shown above is applied with only two very minor differences to calculate the enthalpies of formation of Group 1 and Group 2 metal ions.  $X$ , rather than being the size of an anion, is the “radius” of the space occupied by the electrons detached from the metal atom. In the above expression,  $\Sigma Q_i^2$  is the sum of the squares of the charges on the positive ions and the detached outermost electron(s). For Group 1 metals,  $Q_i^2$  of the positive ion is 1 since each ion has a +1 charge. However,  $Q_i^2$  of the outermost electron is only 0.25 since at any one time only a quarter of the available midpoint sites is occupied. Hence,  $\Sigma Q_i^2$  is equal to  $1+0.25$  (1.25) for all the Group 1 metals. For elements of Group 2,  $Q_i^2$  for the positive ions in all cases is 4 (since they are all dipositive). However, there are 2 different values of  $\Sigma Q_i^2$ . For the first 4 elements, only a third of the sites are occupied by electrons. Hence,  $Q_i^2$  for the electrons is  $(1^2+1^2) \times 0.3333$  and  $\Sigma Q_i^2$  is approximately 4.7. As for barium, since

**Table 2** Observed and calculated work functions.

Element	Structure	Calculated work function(eV)	Observed work function(eV)	Abs % difference
Li	bcc	2.94	2.93	0.5
Na	bcc	2.52	2.36	6.7
K	bcc	2.19	2.29	4.2
Rb	bcc	2.1	2.26	7.3
Cs	bcc	2	1.95	2.6
Mg	hcp	3.4	3.66	7.1
Ca	ccp	2.99	2.87	4.2
Sr	ccp	2.82	2.59	8.9
Ba	bcc	2.67	2.52	5.8
Ti	hcp	4.46	4.33	3.1
V	bcc	4.39	4.3	2.1
Cr	bcc	4.51	4.5	0.3
Mn	bcc	4.36	4.1	6.2
Fe	bcc	4.53	4.74	4.4
Co	ccp	5	5	0
Ni	hcp	4.76	5.2	8.4
Cu	ccp	4.94	4.76	3.7
Zn	hcp	4.59	4.27	7.6
Nb	bcc	4.17	4.33	3.6
Zr	hcp	4.22	4.05	4.3
Mo	bcc	4.29	4.57	6.2
Ru	hcp	4.71	4.71	0
Rh	ccp	4.8	4.98	3.5
Ag	ccp	4.62	4.63	0.1
Cd	hcp	4.28	4.08	4.9
Ta	bcc	4.17	4.3	2.9
W	bcc	4.27	4.55	6.1
Hg	hcp	3.9	4.47	12.9
Pb	ccp	4.17	4.25	1.9

half of the available midpoint sites are occupied at any one time,  $Q_2^2$  for the electrons is  $(1^2+1^2) \times 0.5$ . Hence  $\Sigma Q_2^2$  has a value of 4 plus 1 which equals 5. The calculated values are provided in Table 3. Differences between literature values and those calculated by (3) are less than 10% for all cases.

### The densities of transition metals

The density of a metal is a function of its relative atomic mass and atomic volume. For any positive ion, the higher the number of electrons removed the smaller will be the volume of the ion. For any transition metal in the 3d series, assuming that the electrons in the first two electron shells do not have a great effect on the volume of the metal ion, then the size of the ion is proportional to  $\{(n-x)/n\}$  where  $n$  is the number of 3s, 3p, 4s and 3d electrons in the neutral atom (and 4s, 4p, 5s, and 4d electrons for the

4d series),  $x$  is the number of electrons detached from it. Then simplistically, the atomic volume is  $V=\{k(n-x)/n\}$  where  $k$  is a constant. Since density is mass per unit volume the density of a transition metal can be calculated with the simple expression:

$$D_s = \{[(\text{relative atomic mass}) / \{k(n-x)/n\}]\} k_1 \quad (4)$$

In (4),  $k$  is 30 for the 3d series and 39.5 (a bigger number since 4d ions have a more electron shell) for the 4d series and  $k_1$  is 1.63. Densities calculated by (4) are presented in Table 4. In the above Table, Column 1 lists the elements, Column 2 shows the actual densities of the metals, Column 3 lists the number of detached electrons for each individual metal, Column 4 shows the densities calculated from 4. It is fairly remarkable that the densities calculated from a very simple expression agree fairly well with observed densities as shown in Column 5.

### Discussion

Band theory [22], which is based on quantum mechanics, postulates the existence of energy bands in solids that influence the behavior of electrons. The soft-sphere model of metallic structure can be interpreted as complementing band theory. Metals are malleable because not all available midpoint sites are occupied by electrons. When a metal is twisted or bent, electrons can move from one site to another within a unit cell, allowing the shape of the metal to change without any bonds being broken. Experiment has shown that when sodium is under high pressure the resistance of the metal increases drastically and acts more like an insulator [7] than a conductor of electricity. This behavior cannot be easily explained by the standard "electron sea" model. However, this can be accounted for by the soft-

**Table 3** Enthalpies of formation of  $M^+$  (Group 1) and  $M^{2+}$  (Group 2).

Element (1)	Observed/literature values (2)	Soft-sphere calculated by (3)	Abs % difference (4)
Li	679.55	683.56	0.6
Na	603.37	584.35	3.2
K	507.83	509.26	00.3
Rb	483.95	486.47	00.5
Cs	452.22	464.61	2.7
Be	2980.74	3108.22	4.3
Mg	2335.64	2135.67	8.5
Ca	1913.16	1784.55	6.7
Sr	1778.19	1645.25	7.5
Ba	1648.14	1569.24	4.8

**Table 4** Comparison of calculated and actual densities of 3d and 4d transition metals.

Element (1)	Density (actual) (2)	(x) Nr of detached electrons (3)	Calculated density (4)	Abs % difference (5)
Sc	2.99	1	3.25	8.7
Ti	4.51	2	4.49	0.3
V	6	3	6.08	1.3
Cr	7.15	4	7.75	8.4
Mn	7.3	4	7.57	3.7
Fe	7.87	4	7.9	8.6
Co	8.86	5	9.1	2.7
Ni	8.9	5	8.46	4.9
Cu	8.96	5	8.63	3.7
Zn	7.14	4	6.97	2.8
Y	4.47	1	4.88	9.2
Zr	6.52	2	6.5	0.2
Nb	8.57	3	8.42	1.7
Mo	10.2	4	10.87	6.5
Tc	11	4	10.25	6.9
Ru	12.1	5	12.83	6.1
Rh	12.4	5	12.07	2.6
Pd	12	5	11.66	2.9
Ag	10.5	5	11.13	6
Cd	8.69	4	9.06	4.3

sphere model. When a metal is under high pressure, the shape and size of the unit cell changes. This reduces the volume of the sites occupied by the detached electrons and if the volume is reduced sufficiently the site can no longer be occupied. When the shape of the unit cell changes, the distance between some of the midpoint sites may increase to such an extent, the detached electrons occupying those sites may no longer be able to move from one site to another. Hence, if there are no vacant sites which can facilitate electron movement or if the electrons cannot move between sites in neighboring unit cells the metal becomes an insulator. Assuming that in a metal the positive ions are truly surrounded by a "sea" of delocalized electrons, it is reasonable to assume that the work function of a metal is not significant since electrons from the "electron sea" can move freely to the surface of the metal. However, the work functions of some metals are much higher than some bond dissociation energies and ionization energies. For example, the work function of beryllium is 480.5 kJ/mole and the mean bond dissociation energy of the C-H bond is only 338.4 kJ/mole and that of Ca-Ca is only 16.5 kJ/mole and the first ionization energy of cesium is 3.894 eV (equal to 375.6 kJ/mole). This again demonstrates the flaws of the electron sea description. Since all unit cells in a metal are identical and there are vacant sites which facilitate electron movement, a very small potential difference between the ends of a metal strip or wire can overcome the electrostatic attraction between the positive ions and detached electrons and generate an electron flow along the wire (i.e., an electric current). The attraction between the detached electrons and the positive ions in the unit cell and the energy needed for the detached electrons to jump from one vacant midpoint site in a unit cell to another unit cell give rise to electrical resistance. Metals are good conductors of heat and sound and the "free electron" model suggests that metals show high thermal conductivities due to the presence of the "electron gas" in the metal and a similar explanation is also provided for the conductivity of sound in a metal. It has been calculated that the drift velocity of a "free" electron in copper is about 1 mm/sec [23] whereas the speed of sound in a metal is of the order of thousands of meters per second. The thermal conductivity of a metal is a complex function of temperature and not directly proportional to temperature. For example, at 300 K, the thermal conductivity of silver is 4.29 W/cm K, whereas the thermal conductivity of diamond, which is a covalent solid without an "electron sea" has a thermal conductivity of over 8 W/cm K at this temperature [13]. A metal is a good conductor of heat and sound because of its

density, regular packing and closeness of neighboring particles which allow heat and sound energy to pass quickly from one particle to another in all directions rather than the "electron sea". A catalyst can increase the rate of a reaction by changing the route/way in which the reactants react. The "detached" electrons only occupy sites within the unit cell which means there are very few or no "detached" electrons on the surface of a metal. When reactants are adsorbed onto the surface of a metal new unit cells are formed between the reactants and the metal surface. This allows electrons to flow from the reactants to the surface of the metal and vice versa enabling electron movement between reactants and bond breaking/bond formation to take place. Hence, a new route is provided for the required reaction and increases the reaction rate. When a metal wire with an electric current flowing through it is placed in a transverse magnetic field, a potential difference is developed across the wire at right angles to both the field and the length of the wire. This is known as the Hall effect. It happens because the magnetic field at right angles to the length of the wire creates a force acting on each electron and since, within every unit cell, there are vacant sites between the positive ions for the electrons to occupy, detached electrons can move across at right angles to the length of the wire and congregate into more sites on one side of the wire than the other, thus developing a potential difference across the cross section of the wire and at right angles to the field and length of the wire.

## Conclusion

In contrast to the popular "electron sea" model, we are able to show that, the atomic/metallic radii and enthalpy of formation of the positive metal ions calculated with the alternative model and soft-sphere radii give very good agreement with experimental values. We also showed that the work functions are inverse functions of the soft-sphere radii and the densities of transition metals calculated using the alternative soft-sphere concept agrees well with actual values. The changes in resistance of a metal under pressure can also be interpreted by the alternative model. All of the above provide strong evidence that the alternative model is a more realistic representation of the structure and bonding of metals than the "electron sea" model.

## Statement of Interest

There are not competing interests involved in this work.

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