STRUCTURAL INSIGHTS AT THE ATOMIC LEVEL OF IMPORTANT MATERIALS: Al and Mn as special examples in honor of D. Shechtman

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ABSTRACT

A basic insight into the atomic structures of elements of the Periodic Table are presented in terms of their covalent radii, Bohr radii, nuclear and electron radii and their relation to the Golden ratio. The detailed structures of the quasi crystal forming elements, aluminium and manganese have been chosen here as special examples. At the atomic level, their crystal parameters and bond lengths are shown in detail for the first time and related to the Bohr radii obtained from the first ionization potentials. It is hoped that this work will provide deeper insights into the understanding of the bonding and alloy formation of different materials and help in designing materials for their intended purpose.

Keywords: Atomic radii, Bohr radii, Golden Ratio, Atomic structure, Bond lengths, Aluminium, Manganese.

INTRODUCTION

Over a decade ago, the author[1] arrived at the conclusion that the ground state Bohr radius, a_B of a hydrogen (H) atom obtained from its ionization potential (I_H) is divided at the Golden point into two Golden sections, a_{e-} and a_{p+} pertaining to the electron (e^-) and proton (p^+), respectively. These are expressed by the equations,

$$a_B = e/2\kappa I_H = a_{e-} + a_{p+} \; ; \; a_{p+} = (a_B/\phi^2) \text{ and } a_{e-} = (a_B/\phi) = \phi a_{p+} \qquad (1a\text{-}c)$$

where e is the charge, κ is the electrical permittivity of vacuum, $e/2\kappa = 7.1998$ Å/eV and $\phi = (1+5^{1/2})/2) = 1.618$ is the Golden ratio, also called The Divine Ratio.

The bond length d(HH) in the hydrogen molecule was shown to be the diagonal of a square with the Bohr radius as a side. Since the latter has two Golden sections, d(HH) is also divided into two Golden sections which form the anionic and cationic radii of H. The cationic radius, $d(H^+) = d(HH)/\phi^2 = 0.28$ Å is exactly the value suggested empirically by Pauling[2] to explain the bond lengths in hydrogen halides (HX) and it also explained the bond lengths in alkali metal hydrides (MH). This cascaded into the findings[1] that the bond length d(AA) between two atoms (A) of the same kind is divided at the Golden point into two Golden sections, $d(A^-)$ and $d(A^+)$, which form the anionic (A^-) and cationic (A^+) radii of atoms as shown below,

$$d(AA) = 2d(A) = d(A^-) + d(A^+) \qquad (2a)$$

$$d(A^+) = d(AA)/\phi^2 \text{ and } d(A^-) = d(AA)/\phi \qquad (2b,c)$$

where $d(A) = d(AA)/2$ is the covalent radius. The radii increase in the order, $d(A^+) > d(A) > d(A^-) = (2/\phi^2) > 1 > (2/\phi) = 0.764 > 1 > 1.236$. *Note*: the symbol d is used here for covalent radii since they are apportioned distances.

In the case of the ionic crystals of alkali halides (MX), it was shown[1] that the Golden ratio based cationic (M^+) and anionic (X^-) radii, $d(M^+) = d(MM)/\phi^2$ and $d(X^-) = d(XX)/\phi$ respectively, add up to give the exact crystal ionic distances d(MX), where the inter-atomic bond length, d(MM) = a, the lattice parameter for the bcc lattice of the alkali metals (M) and d(XX) is the bond length in the diatomic halogen (X) molecules. It was gradually found that bond lengths between any two atoms, d(AB), in many inorganic, organic and biological molecules can be expressed as the sum of the radii of A and B, whether they be covalent or ionic. A whole series of over 20 contributions/publications[3-24] followed the above findings.

Amongst these, it was also shown[8,15,17] that the covalent atomic radii, d(A) and various other radii of atoms (A) of many Group A elements vary linearly with their Bohr radii, $a_{B,A}$ obtained from their first ionization potentials (I_1), as in the case of hydrogen,

$$a_{B,A} = e/2\kappa I_1 \quad (3)$$

In[17] the covalent atomic radii obtained from lattice parameters and the Bohr radii ($a_{B,A}$) for all the elements of the Periodic Table were shown to be related by a simple function of ϕ:

$$d(A)/a_{B,A} = K_\phi = \tan\theta \quad (4a,b)$$

PRESENT WORK AND RESULTS

In this article, data from[17] have been used. It can be seen in the data in[16] that in each Group, the ratio K_ϕ increases with increasing d(A). Hydrogen has the lowest value while the inert gases and mercury have high values around 2.

Fig. 1 shows the sizes of the covalent atomic radii of atoms relative to their Bohr radii for some arbitrary values of K_ϕ.

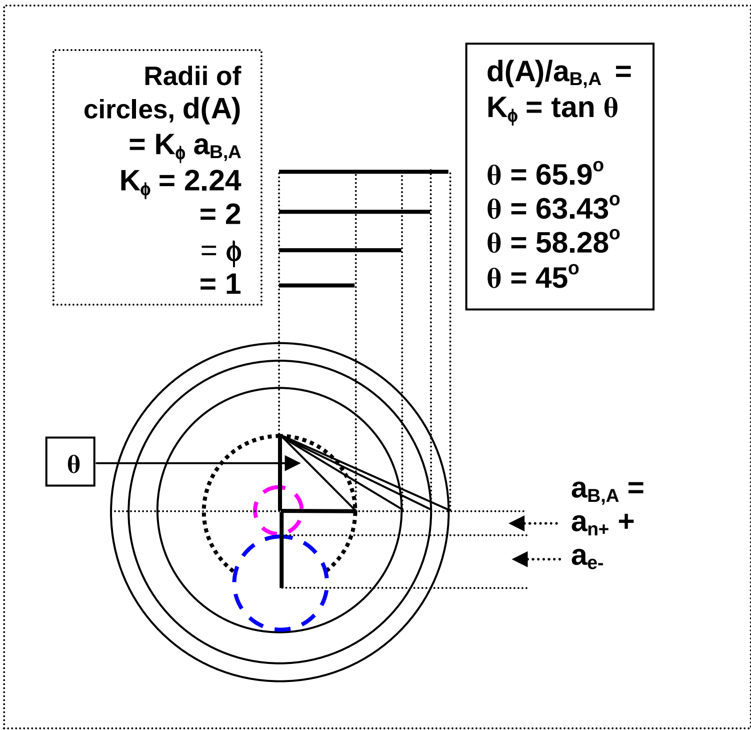

Fig. 1. Covalent radii, d(A) = d(AA)/2 of atoms relative to their Bohr radii ($a_{B,A}$) for some chosen values of $K_\phi = d(A)/a_{B,A} = \tan\theta$.

The case of great interest for the author was to find out the atomic structures of Al and Mn, which form alloys and quasi crystals with the Golden ratio in their lattice structures.

The detailed structure of Aluminium is shown in Fig 2. The values[25] of the fcc cell parameters, covalent radius d(A) = 1.43 Å and Bohr radius[17] are given in Fig.2. The ratio, $K_\phi = d(A)/a_{B,A} = (1+1/2\phi^2) = 1.19$. The cell parameter, $a = b = c = 4.05$ Å $= 2^{1/2}d(AA) = 2^{3/2}(a_{B,A}+a_{e-}/2\phi)$. Note that two adjacent atoms of the same radii make an angle $\sin^{-1}(2/5^{1/2}) = 63.43^0$ a shown in Fig. 2, where $5^{1/2}/2 = \phi - 1/2$.

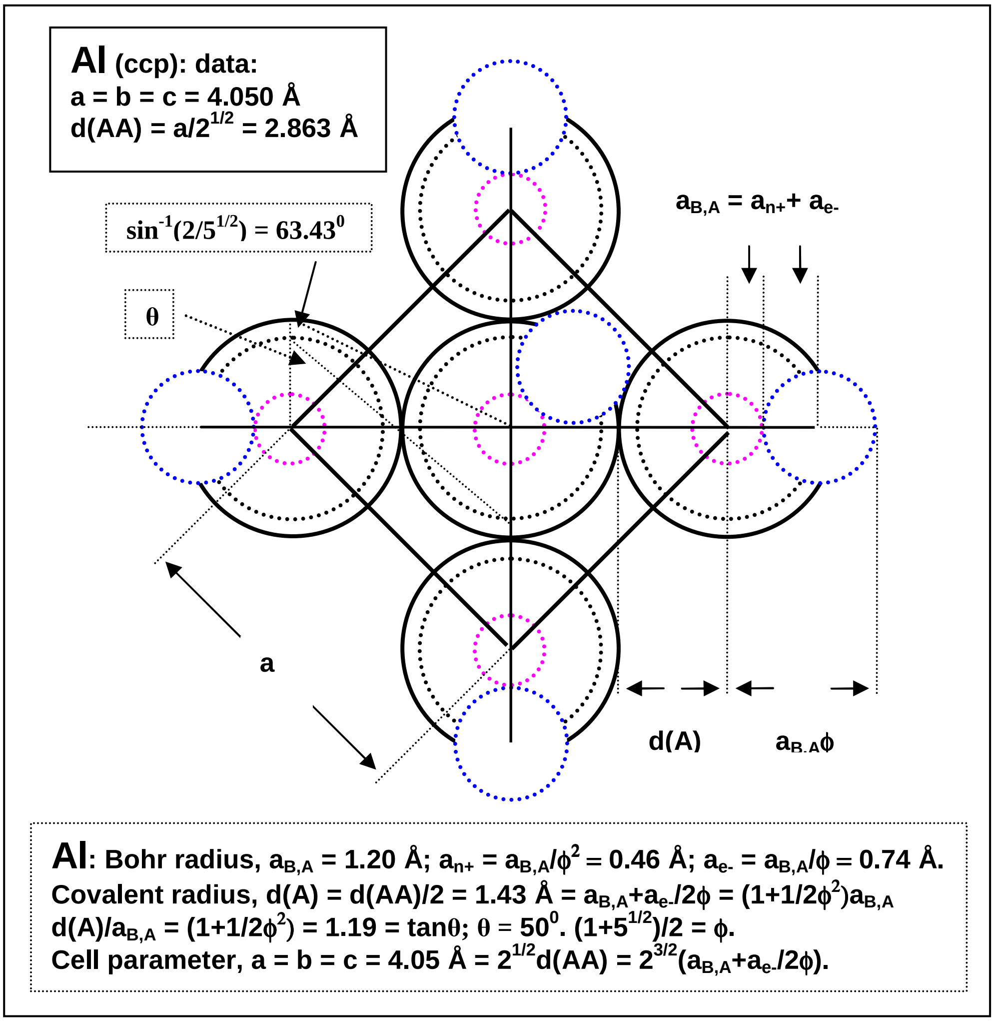

Fig. 2. Structure at the atomic level of Aluminium. The cell parameter, a = b = c is the diagonal of a right angled triangle with sides equal to the bond length, d(Al-Al). $a_{B,A}$ is the Bohr radius of Al and a_{n+} and a_{e-} are the radii of its nucleus and electron.

In the case of manganese, the cell parameters[25] and the bond length d(Mn-Mn) = 2.73 Å are as given in the Fig. 3. It is striking to see that the diagonal, $2^{1/2}$d(Mn-Mn) of a square with d(Mn-Mn) as the sides is exactly $4a_{B,A}$ = 3.87 Å, the diameter of two Bohr circles. The central circle is a hole with Bohr radius.

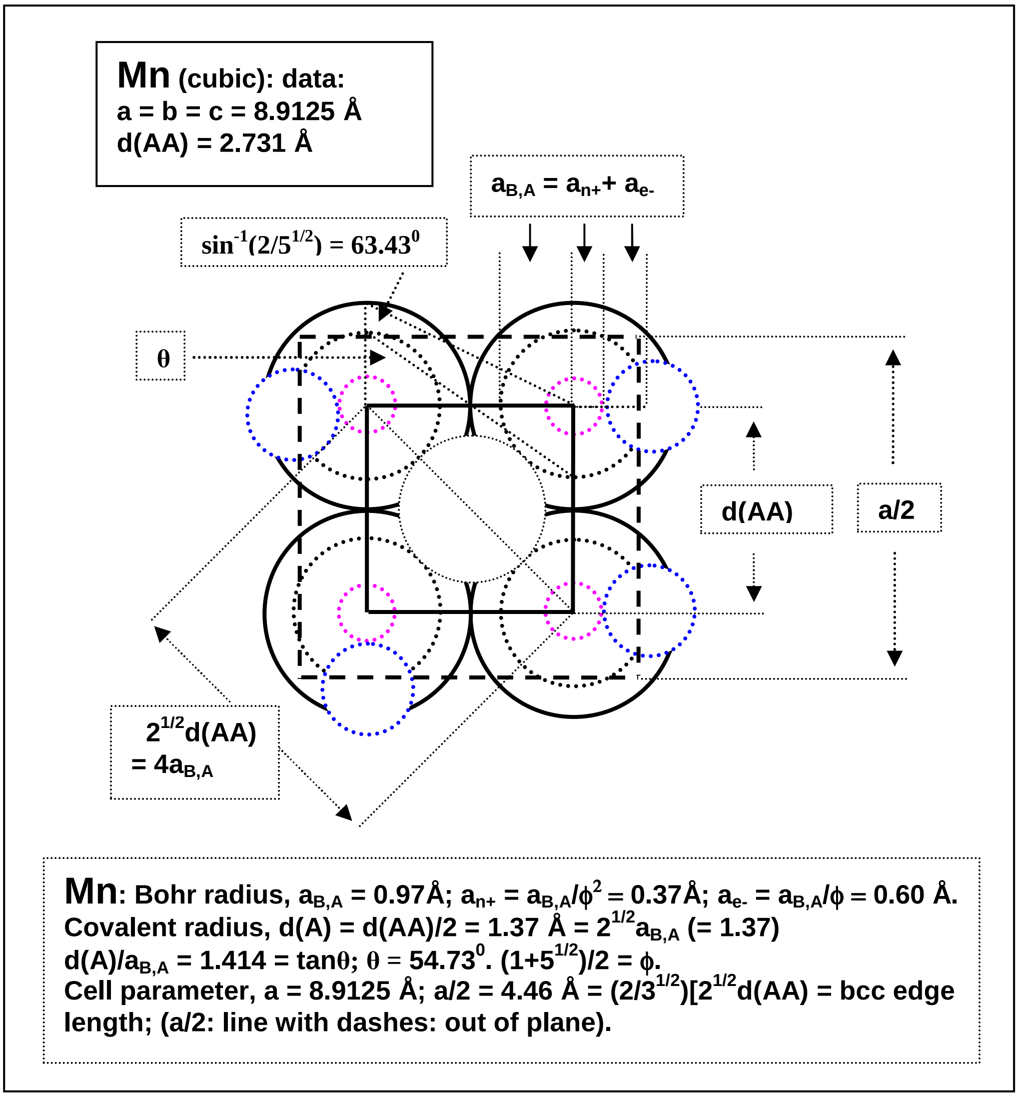

Fig. 3. Structure at the atomic level of Manganese. The cell parameter, a = b = c = 8.9125Å. The distance a/2 is of a body center cube with the center to edge distance equal to $2^{1/2}$d(Mn-Mn), which is the diagonal of the square with sides equal to d(Mn-Mn). $a_{B,A}$ is the Bohr radius and a_{n+} and a_{e-} are the radii of its nucleus and electron.

Half the cell parameter, a/2 is the edge length of a bcc structure, with the center to edge distance equal to the diagonal of the square, $2^{1/2}$d(Mn-Mn) = $4a_{B,A}$.

It is hoped that the above structures of Al and Mn can be put together to construct the 3D structures of Al-Mn alloys and explore their relation to the Golden ratio.

Similarly, the structures at the atomic level of other materials can be elucidated and materials can be chosen for their desired purposes.

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