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ONE-CELL-STATE METHOD FOR DETERMINATION OF ELECTRONIC STRUCTURE OF INTERMETALLIC COMPOUNDS①

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ABSTRACT The basic-cell-state which can be used to describe the characteristic property of intermetallic compounds was constructed on the basis of new development in the basic-atom-state, and also a new method, one-cell-state-method, was established in terms of the basic-cell-state. To take Al_3Li as an example, how to use the new method to determine the electronic structure of the cell in intermetallic compounds is briefly introduced. The new method is valid for determination and analysis of the interatomicic charge transfer and the component of ionicity in chemical bond.

Key words one-cell-state method intermetallic compound electronic structure charge transfer Al_3Li

1 INTRODUCTION

In recent years, the Pauling's valence bond (VB) theory has been made a great progress in designing and determining the atomic state, and in establishing the relation among the atomic states as well as crystal structure and physical property. First, Yü[1] developed the Pauling's valence bond theory to calculate the electronic structure of crystal and set up the two-hybrid-state model. Then, Lü[2] established the relation between bond parameter and crystal cohesive energy. Second, Xie determined the corresponding relation between electronic structure of crystal and characteristic properties (spacing constant and cohesive energy). Furthermore, he proposed an one-atom-state method[3] and gave a new many-atom-interaction potential[4] which make it possible to further analyse the electronic structure of pure metals and alloys as well as physical properties. In this paper, based on the one-atom-state (OAS) method of pure metal, we develope and establish a new method, one-cell-state (OCS) method, which can be used to determine the electronic structure of intermetallic compounds. To take Al_3Li as an example, we briefly introduce how to construct the basic-cell-state (BCS) and how to use the new method to determine the electronic structure of intermetallic compounds.

2 PRINCIPLE OF BCS CONSTRUCTION

Xie has given the construction principle of basic-atom-state (BAS) of pure metals in OAS method[3]. However, as far as intermetallic compounds are concerned, because they are composed of different kinds of atoms, and there are not only covalence bond among atoms, but also ionic bond due to the charge transfer between atoms, their chemical bond are rather complicated. The unit that reflects the characteristic of intermetallic compounds are not the atom, but the primary cell or crystal cell. Considering the symmetry of crystal, we choose the crystal cell as the characteristic unit of crystal. Here we briefly call

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it as the one-cell.

On the principles basis of BAS construction, the principles of BCS construction are as below:

1) The BCS are a composite state which is composed of some BAS of all atoms belonging to a cell. 2) The cell should maintain electroneutrality, i. e, the total electronic number in cell are equal to the sum of electronic number in neutral atoms belonging to the cell. 3) There are not only charge transfer in intra-atomic energy level, but also in interatom, however, no charge transfer between two cell, or to say, the charge transfer in or out in a cell is balanced. 4) The interatomic charge transfer in a cell is usually the s or p electrons. Because of the localization of d electrons, they do not take part in charge transfer in general case. While in the case of s-d or p-d electronic hybridization, d electrons will refer to charge transfer. 5) The quantity of interatomic charge transfer in BCS are the integral electron charge. The quantity of charge transfer in or out for equavalent atoms is equal. 6) According to it whether there is interatomic charge transfer in a cell or not, we can divide the BCS into two kinds. The one that there are interatomic charge transfers in cell is called the polar-basic-cell-state (PBCS), the other that no interatomic charge transfers is called the upolar-basic-cell-state or neutral-basic-cell-state (NBCS).

According to the principle of BCS construction given above, we can design some BCS. For example, if there are four kinds of atom in a cell, each kind of atom has one atom belonging to the cell, and for the sake of simplicity, here we only consider the case that there are only s and p electrons in outer shell of atoms; and the s electrons can be divided into covalence electrons s_c and near free electrons s_f which are only limited in s state; the p electrons are only the covalence electrons p_c; and the four kinds of atoms in a cell are designated by A, B, C, D, then the BCS φ^{cell} can be written as:

$$\begin{aligned}\varphi_k^{\text{cell}} = [&(s_f^{\alpha},\ s_c^{\beta},\ p_c^{\gamma})_A(s_f^{\alpha'},\ s_c^{\beta'},\ p_c^{\gamma'})_B\\ &(s_f^{\alpha''},\ s_c^{\beta''},\ p_c^{\gamma''})_C(s_f^{\alpha'''},\ s_c^{\beta'''},\ p_c^{\gamma'''})_D]_k\end{aligned} \tag{1}$$

where the uppermark α, β, γ, …, α''', β''', γ''' are integral numbers and denote the electronic numbers occupying the outer shell s and p orbital. The undermark A, B, C, D denote the atoms in the cell. The undermark k means the kth BCS. The electroneutrality in cell requires

$$\begin{aligned}&(\alpha+\beta+\gamma)+(\alpha'+\beta'+\gamma')+\\ &(\alpha''+\beta''+\gamma'')+\\ &(\alpha'''+\beta'''+\gamma''')=Q_0\end{aligned} \tag{2}$$

where Q_0 denotes of the total outer shell electronic numbers in the neutral cell. The outer shell electronic numbers of neutral atoms in the cell are respectively denoted by q_A, q_B, q_C, q_D. If no interatomic charge transfer in the cell, i. e,

$$\begin{aligned}&\alpha+\beta+\gamma=q_A,\quad \alpha'+\beta'+\gamma'=q_B,\\ &\alpha''+\beta''+\gamma''=q_C,\quad \alpha'''+\beta'''+\gamma'''=q_D\end{aligned} \tag{3}$$

then those BCS which satisfied the conditions of the atomic electroneutrality in equation (3) is called the neutral BCS or NBCS, expressed by φ_k^0. If one or more equations in (3) formula are not satisfied, i. e, there is at least one atom in the cell which does not obey electroneutrality in atoms, but the equation $q_A+q_B+q_C+q_D=Q_0$ is still held, then these BCS are called the polar-basic-cell-state (PBCS), expressed by φ_k^*. If there are three kinds of atoms are equivalent in the cell (supposing A, B, C atoms are equivalent), then the BCS can be briefly written as

$$\varphi_k^{\text{cell}} = [(s_f^{\alpha},\ s_c^{\beta},\ p_c^{\gamma})_A^3(s_f^{\alpha'},\ s_c^{\beta'},\ p_c^{\gamma'})_D] \tag{4}$$

and its supplementary condition is

$$3(\alpha+\beta+\gamma)+(\alpha'+\beta'+\gamma')=Q_0$$

3 BCS CONSTRUCTION OF Al_3Li

According to the principle of BCS construction given above, here we take the intermetallic compound Al_3Li with $L1_2$ crystal structure as an example, to show how to design the BCS. Because there are three equivalent Al atoms and one equivalent Li atom in Al_3Li, and each neutral Al or Li atom has respectively three outer valence electrons or one outer valence electron, however here we only consider the s and p state of electrons in atoms, then the BCS of Al_3Li can be written as

$$\varphi_k^{\text{cell}} = [(s_f^{\alpha},\ s_c^{\beta},\ p_c^{\gamma})_{\text{Al}}^{3} \cdot (s_f^{\alpha'},\ s_c^{\beta'},\ p_c^{\gamma'})_{\text{Li}}]_k$$

or briefly written as

$$\varphi_k^{\text{cell}} = [(\alpha,\ \beta,\ \gamma)_{\text{Al}}^{3}(\alpha',\ \beta',\ \gamma')_{\text{Li}}]_k \tag{5}$$

where α or α', β or β', γ or γ' denote respectively the occupation number of near free electron s_f and covalence electrons s_c in s orbital, as well as covalence electrons p_c in p orbital. The occupation numbers of the s and p electrons obey the Pauli principle. Thirty BCSs are given in Table 1, in which fifteen are NBCS and other fifteen are PBCS (here only considering the case of one electron from one Al atom transfer to Li atom).

Table 1 NBCS φ_k^0 and PBCS φ_k^* of Al_3Li

φ_k^0	Outer shell electron distribution	φ_k^*	Outer shell electron distribution
φ_1^0	$(0, 0, 3)_{\text{Al}}^3(1, 0, 0)_{\text{Li}}$	φ_1^*	$(1, 0, 1)_{\text{Al}}^3(1, 0, 3)_{\text{Li}}$
φ_2^0	$(0, 0, 3)_{\text{Al}}^3(0, 1, 0)_{\text{Li}}$	φ_2^*	$(1, 0, 1)_{\text{Al}}^3(2, 0, 2)_{\text{Li}}$
φ_3^0	$(0, 0, 3)_{\text{Al}}^3(0, 0, 1)_{\text{Li}}$	φ_3^*	$(0, 1, 1)_{\text{Al}}^3(1, 0, 3)_{\text{Li}}$
φ_4^0	$(1, 0, 2)_{\text{Al}}^3(1, 0, 0)_{\text{Li}}$	φ_4^*	$(0, 1, 1)_{\text{Al}}^3(2, 0, 2)_{\text{Li}}$
φ_5^0	$(0, 1, 2)_{\text{Al}}^3(1, 0, 0)_{\text{Li}}$	φ_5^*	$(1, 0, 1)_{\text{Al}}^3(0, 2, 2)_{\text{Li}}$
φ_6^0	$(1, 0, 2)_{\text{Al}}^3(0, 1, 0)_{\text{Li}}$	φ_6^*	$(1, 0, 1)_{\text{Al}}^3(0, 1, 3)_{\text{Li}}$
φ_7^0	$(0, 1, 2)_{\text{Al}}^3(0, 1, 0)_{\text{Li}}$	φ_7^*	$(0, 1, 1)_{\text{Al}}^3(0, 2, 2)_{\text{Li}}$
φ_8^0	$(1, 0, 2)_{\text{Al}}^3(0, 0, 1)_{\text{Li}}$	φ_8^*	$(0, 1, 1)_{\text{Al}}^3(0, 1, 3)_{\text{Li}}$
φ_9^0	$(0, 1, 2)_{\text{Al}}^3(0, 0, 1)_{\text{Li}}$	φ_9^*	$(1, 0, 1)_{\text{Al}}^3(0, 0, 4)_{\text{Li}}$
φ_{10}^0	$(0, 2, 1)_{\text{Al}}^3(1, 0, 0)_{\text{Li}}$	φ_{10}^*	$(0, 1, 1)_{\text{Al}}^3(0, 0, 4)_{\text{Li}}$
φ_{11}^0	$(0, 2, 1)_{\text{Al}}^3(0, 1, 0)_{\text{Li}}$	φ_{11}^*	$(1, 1, 0)_{\text{Al}}^3(1, 0, 3)_{\text{Li}}$
φ_{12}^0	$(0, 2, 1)_{\text{Al}}^3(0, 0, 1)_{\text{Li}}$	φ_{12}^*	$(1, 1, 0)_{\text{Al}}^3(2, 0, 2)_{\text{Li}}$
φ_{13}^0	$(2, 0, 1)_{\text{Al}}^3(1, 0, 0)_{\text{Li}}$	φ_{13}^*	$(1, 1, 0)_{\text{Al}}^3(0, 2, 2)_{\text{Li}}$
φ_{14}^0	$(2, 0, 1)_{\text{Al}}^3(0, 1, 0)_{\text{Li}}$	φ_{14}^*	$(1, 1, 0)_{\text{Al}}^3(0, 1, 3)_{\text{Li}}$
φ_{15}^0	$(2, 0, 1)_{\text{Al}}^3(0, 0, 1)_{\text{Li}}$	φ_{15}^*	$(1, 1, 0)_{\text{Al}}^3(0, 0, 4)_{\text{Li}}$

4 DETERMINATION OF ELECTRONIC STRUCTURE Al_3Li

4.1 BCS parameter

In the new developed one-cell-state (OCS) method, the electronic structure of intermetallic compounds can be illustrated by OCS ϕ_c which consists of some BCS φ_k^{cell} as below:

$$\phi_c = \sum_k c_k \varphi_k^{\text{cell}} \tag{6}$$

in some BCS of Al_3Li ($L1_2$) intermetallic compounds have been given in Table 1.

If $s_{c,k}^{\text{Al}}$, $s_{c,k}^{\text{Li}}$ and $p_{c,k}^{\text{Al}}$, $p_{c,k}^{\text{Li}}$ denote, respectively, the number of covalence electrons of the outer s and p shell in Al and Li atoms in the kth BCS; $s_{f,k}^{\text{Al}}$ and $s_{f,k}^{\text{Li}}$ denote respectively the near free electrons in the outer s orbital in Al and Li atoms, then the parameter s_c^{cell}, p_c^{cell}, s_f^{cell} of one cell state can be obtained from below expression:

$$\left.\begin{aligned}
s_c^{\text{cell}} &= \sum_k c_k s_{k,c}^{\text{cell}} = \sum_k c_k (s_{k,c}^{\text{Li}} + 3s_{k,c}^{\text{Al}}),\\
p_c^{\text{cell}} &= \sum_k c_k p_{k,c}^{\text{cell}} = \sum_k c_k (p_{k,c}^{\text{Li}} + 3p_{k,c}^{\text{Al}})\\
N_f &= s_f^{\text{cell}} = \sum_k c_k s_{k,f}^{\text{cell}} = \sum_k c_k (s_{k,f}^{\text{Li}} + 3s_{k,f}^{\text{Al}}),\\
N_c &= s_c^{\text{cell}} + p_c^{\text{cell}},\\
N_T^V &= N_c + N_f
\end{aligned}\right| \tag{7}$$

$$\left.\begin{aligned}
R^{\text{Li}} &= \sum_k c_k R_k^{\text{Li}},\quad R^{\text{Al}} = \sum_k c_k R_k^{\text{Al}},\\
R_k^{\text{Li}} &= 1.115 - 0.12\,\delta_k^{\text{Li}},\\
R_k^{\text{Al}} &= 1.308 - 0.25\,\delta_k^{\text{Al}},\\
\delta_k^{\gamma} &= [p_k^c/(p_k^c + s_k^c + s_k^f)]_{\gamma}
\end{aligned}\right| \tag{8}$$

where γ in last formula in equation (8) denote the Al or Li atoms. Here R_k^{γ}, which is the single-bond radius of Al and Li atom in the kth BCS, can be obtained from Pauling's equation[10] slightly modified by author.

4.2 Bond parameter

The bond parameters of ordered Al_3Li intermetallic compound are expressed as below:

$$\left.\begin{aligned}
&\text{Al-Li bond},\ I_1 = 24,\\
&r_1 = a/\sqrt{2} = R^{\text{Al}} + R^{\text{Li}} - \beta \lg n_1\\
&\text{Al-Al bond},\ I_2 = 24,\\
&r_2 = a/\sqrt{2} = 2R^{\text{Al}} - \beta \lg n_2\\
&\text{Al-Al bond},\ I_3 = 18,\\
&r_3 = a = 2R^{\text{Al}} - \beta \lg n_3\\
&\text{Li-Li bond},\ I_4 = 6,\\
&r_4 = a = 2R^{\text{Li}} - \beta \lg n_4\\
&N_c = I_1 n_1 + I_2 n_2 + I_3 n_3 + I_4 n_4
\end{aligned}\right| \tag{9}$$

where $\beta = 0.6$ is determined by Pauling, N_c are the total numbers of covalence electrons, n_1,

n_2, n_3, n_4 are the bond strength, and I_1, I_2, I_3, I_4 are the numbers of the same kind of bond, and r_1, r_2, r_3, r_4 are the bond length. The a is the spacing constant.

To s-p electronic hybridization of the same kind of atoms, the bond capacity can be expressed as

$$f = \sqrt{\alpha} + \sqrt{3\delta},\quad \alpha = s^c/N_T^V,\quad \delta = p^c/N_T^V, f' = \sqrt{2\alpha'},\quad \alpha' = N^f/N_T^V = s_f/N_T^V \tag{10}$$

where N_T^V is the total valence electron numbers, f is the bond capacity of covalence electron for Al or Li atoms, f' is the bond capacity for near free electrons.

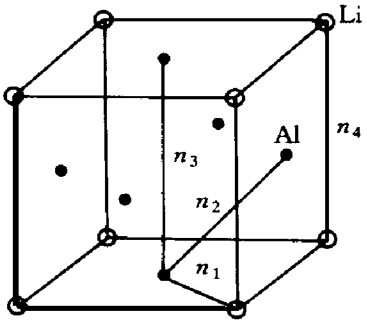

Fig. 1 Al_3Li crystal structure

4. 3 Characteristic property of crystal

To intermetallic compounds with the $L1_2$ structure, the relation between the spacing constant and atomic state of crystal is

$$\alpha = \beta\lg\{ [I_1 \times 10^{(R_1+R_2+a(1-1/\sqrt{2}))/\beta} + I_2 \times 10^{(2R_1+a(1-1/\sqrt{2}))/\beta} + I_3 \times 10^{2R_1/\beta} + I_4 \times 10^{2R_2/\beta}]/N_c\} \tag{11}$$

where R_1 and R_2 denote the single-bond radius of Al and Li atoms respectively. Since I_1, I_2, I_3, I_4 and β are the known constants, so if the atomic state are determined, i. e, the one-cell-state is determined, R^{Al}, R^{Li}, N_c can immediately be determined too. Then similar to the demonstration in Ref. [6], we can easily know the corresponding spacing constant is also solely determined.

The general cohesive energy formula of intermetallic compounds is given in Ref. [7], we can easily derive the detail formula of Al_3Li cohesive energy as below (unit: kJ/mol):

$$\begin{aligned} E_c = & [8.464\bar{B}_{\mathrm{Al\text{-}Li}} \cdot n_1 \cdot \bar{F}_{\mathrm{Al\text{-}Li}} + \\ & b_{\mathrm{Al}} \cdot (8.464n_2 + 4.489n_3) \cdot f_{\mathrm{Al}} + \\ & 1.496b_{\mathrm{Li}} \cdot n_4 \cdot f_{\mathrm{Li}} + \\ & 0.3099\bar{B}'_{\mathrm{Al\text{-}Li}} \cdot N_f \cdot f'] - \\ & [72.29 \times \{a(n_e)^3 + b(\Delta n_e)^2 + \\ & c(\Delta n_e)\} \times e^{-(|\Delta n_e|+0.693)}] + \\ & [5.765 \times (3 \times \Delta n_e) \times y \times \\ & e^{-(3|\Delta n_e|+0.693)}] \end{aligned} \tag{12}$$

The first square brackets in equation (12) denote the bonding energy, where $\bar{B}_{\mathrm{Al\text{-}Li}}$, b_{Al}, b_{Li}, $\bar{B}'_{\mathrm{Al\text{-}Li}}$ are related to the effect of outer shell electrons screening nuclear charge and here their values are $b_{\mathrm{Al}} = 191.5$, $b_{\mathrm{Li}} = 490.5$, $\bar{B}_{\mathrm{Al\text{-}Li}} = \sqrt{b_{\mathrm{Al}} \cdot b_{\mathrm{Li}}} = 306.5$, $\bar{B}'_{\mathrm{Al\text{-}Li}} = \sqrt{b_{\mathrm{Al}}^3 \cdot b_{\mathrm{Li}}} = 243$, and f_{Al}, f_{Li}, f', $\bar{F}_{\mathrm{Al\text{-}Li}}$ can, respectively, expressed as below:

$$\begin{aligned} f_{\mathrm{Al}} &= \sqrt{\alpha_{\mathrm{Al}}} + \sqrt{3\delta_{\mathrm{Al}}}, \\ f_{\mathrm{Li}} &= \sqrt{\alpha_{\mathrm{Li}}} + \sqrt{3\delta_{\mathrm{Li}}}, \\ f' &= \sqrt{2\alpha'}, \\ \bar{F}_{\mathrm{Al\text{-}Li}} &= \frac{1}{2}(f_{\mathrm{Al}} + f_{\mathrm{Li}}) \end{aligned} \tag{13}$$

the second square bracket in equation (12) denote the ionization energy, and the third brackets denote the affinity energy. The coefficient value of a, b, c in equation (12) which can be got from Ref. [8], are respectively -1.68, 8.46 and -0.79, and Δn_e denotes the charge transfer from Al atom to Li atom ($\Delta n_e > 0$), and y is the chemical affinity for Li atom which is given in Ref. [8], i. e, $y = 0.618$, the n_1, n_2, n_3 and n_4 can be derived from equation (9).

4. 4 Selection and determination of hybridization state

From equation (11) and (12), we can get any characteristic property of pseudo-crystals which are composed of a BCS or of some BCS combination. If the normalization condition of coefficient c_k in equation (6) considered, the combination of three or more BCS is needed in general. For example, through the proper selection, if the characteristic property of BCS φ_n, φ'_n and φ''_n satisfied the relation as $E_n < E_{n'} <$

E_n'' and $a_n > a_n' > a_n''$, and furthermore $a_n > a^{\mathrm{Exp}} > a_n''$ and $E_n < E_c^{\mathrm{Exp}} < E_n''$($a^{\mathrm{Exp}}$, E_c^{Exp} are experiment value or truth value), then we can use the computer to build the isograms of a^{Exp} and E_c^{Exp}. Both the isograms of a^{Exp} and E^{Exp} can be obtained, it proves that we can not determine the electronic structure of crystal only by lattice spacing constant or cohesive energy property. The two isogram of a^{Exp} and E_c^{Exp} have only one cross point, this tells us that a group characteristic properties correspond to a crystal state. Fig. 2 shows the three BCS hybridization.

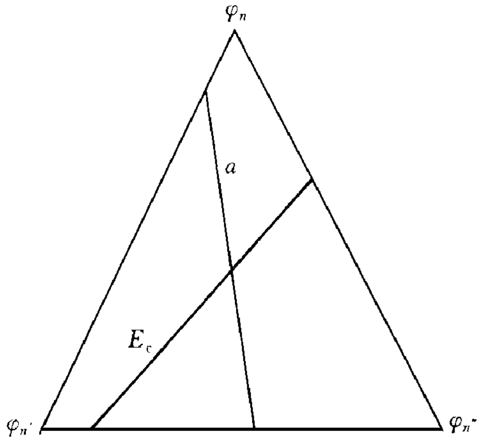

Fig. 2 Characteristic property of three state hybridization of pseudo-crystal

In actual procedure of determining the electronic structure, noting that the charge transfer is much less in intermetallic compounds, i. e., ionic bond are a little part of chemical bond of intermetallic compound crystal and the PBCS will take a small part in one-cell-state (OCS), so we can do first to choose one suitable PBCS and one NBCS to make two state hybridization to get a "new" BCS $\overline{\varphi}_n$, then take $\overline{\varphi}_n$ with two other suitable NBCS $\varphi_{n'}$ and $\varphi_{n''}$ to make three state hybridization and still follow procedure of determining electronic structure in three state hybridization shown in Fig. 2. Finially we can easily determine the electronic structure by that the theory value of characteristic property are the most possible in agreement with that of experiment. The combintion of φ_5^0, φ_9^0, φ_{13}^0 and φ_1^* states are the best combination for one-cell-state (OCS) of Al_3Li intermetallic compounds crystal. The electronic structure of Al_3Li are

$$[(s_f)^{0.56}(s_c)^{0.85}(p_c)^{1.44}]_{\mathrm{Al}}^3 \bullet$$
$$[(s_f)^{0.48}(p_c)^{0.97}]_{\mathrm{Li}}$$

which are in agreement with the result calculated by TBLMTO method[9]. The cell state parameters and characteristic property of Al_3Li are shown in Table 2.

To determine the electronic structure of intermetallic compound with a complicated crystal structure and characteristic property, usually more than three state combinations are needed in order to get an accurate description for electronic structure. In this case, the detailed procedure for determine the electronic structure are still similar to that shown in Fig. 2, but other characteristic properties, such as, magnetic moment, conduction, and anisotropic characteristic of mechanics properties of crystal should be required to consider. The new OCS method given above can also be used to determine the electronic structure of NiAl, TiAl, Cu_3Au, Fe_4N *et al* intermetallic compounds. These results are in good agreement with the experiments, and many physical properties of these material can be well explaination with these results got by the new method. All these results will be reported elsewhere.

4.5 The charge transfer and ionicity

Although Al and Li are both simple metals (no *d* electrons), they are chemically rather different due to their atomic size, valency and electronegativity. So when Al, Li atom combine to form intermetallic compounds, there will be charge transfer between Al and Li atoms in Al_3Li, and the Al-Li covalence bond will have a small component of ionic bond. Following the Pauling's empiric formula[10], we know that there are about 7% ionic bond in Al-Li covalence bond. While using the electronic structure results in Table 2, we can see about 2.85 electrons in the outer shell of Al atom, about 1.45 valence electrons in Li atom and obviously each Al atom transfers 0.15 electrons to Li atom in one cell. The Al-Li bond strength n_1 by our calculation is about 0.14 in Table 2, hence each Al-Li bond

Table 2 Cell state papameters, bond papameters and properties of Al_3Li

Coefficient	c_5	c_9	c_{13}	c_1^*	Bond parameters	r_1/ Å	r_2/ Å	r_3/ Å	r_4/ Å
	0.0464	0.5228	0.2823	0.1485		2.8256	2.8256	3.9961	3.9961
State parameters	s_f^{Al}	s_c^{Al}	p_c^{Al}	n_T^{Al}		n_1	n_2	n_3	n_4
	0.56	0.85	1.44	2.85		0.1401	0.2021	0.0023	0.0011
	R^{Al}	s_f^{Li}	s_c^{Li}	p_c^{Li}	Theoretical value	a / Å		E_c / (kJ·mol^{-1})	
	1.204	0.48	0.00	0.97		3.9961		291.3	
	n_T^{Li}	R^{Li}	N_c^{cell}	N_T^{cell}	Experimental value	a / Å		* E_c / (kJ·mol^{-1})	
	1.45	1.109	7.84	10.00		4.010		291.8	

* Upto now any accurate experimental result E_c^{Exp} of Al_3Li have not been reported, so here the optimum theoretical result instead of the experimental result E_c^{Exp} are used to determine the atomic state. See in Ref. [8]

shares the charge transfer electrons is about $3 \times 0.15/24 \approx 0.0187$, and then the electron transfer quautity in Al-Li bond will take the part about $0.0187/0.14 \approx 13\%$. This quantity can be used to estimate the ionicity in Al-Li covalence bond, so we think that the ionicity in Al-Li covalence bond are about 10%, a little greater than the result obtain by Paulings empiric formula. Here we should take note that the charge transfer is from Al atom with greater electronegativity to Li atom with smaller electronegativity. It shows that the bond capacity of valence electrons in Li atom is very weak. Hence when the interametallic compound is formed, the charge transfer from Al atom to Li atom is needed, in order to form a stronger Al-Li bond. So there are some components of ionic bond in Al-Li covalence bond.

5 CONCLUSION

The OCS method which is on the base of new development in OAS method can be used to determine the electronic structure of intermetallic compounds, especially, it is valid for analysing the interatomic charge transfer as well as ionicity of chemical bond in intermetallic compounds.

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