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Atomic bonding and mechanical properties of Al-Mg-Zr-Sc alloy①

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Abstract: The valence electron structures of Al-Mg alloy with minor Sc and Zr were calculated according to the empirical electron theory(EET) in solid. The results show that because of the strong interaction of Al atom with Zr and Sc atom in melting during solidification, the Al_3Sc and $Al_3(Sc_{1-x}Zr_x)$ particles which act as heterogeneous nuclear are firstly crystallized in alloy to make grains refine. In progress of solidification, the Al-Sc, Al-Zr-Sc segregation regions are formed in solid solution matrix of Al-Mg alloy owing to the strong interaction of Al atom with Zr, Sc atoms in bulk of alloy, so in the following homogenization treatment, the finer dispersed Al_3Sc and $Al_3(Sc_{1-x}Zr_x)$ second-particles which are coherence with the matrix are precipitated in the segregation region. These finer second-particles with the strong Al—Zr, Al—Sc covalent bonds can strengthen the covalent bonds in matrix of the alloy, and also enhance the hardness and strength of Al-Mg alloy. Those finer second-particles precipitated in interface of sub-grains can also strengthen the covalence bonds there, and effectively hinder the interface of sub-grains from migrating and restrain the sub-grains from growing, and cause better thermal stability of Al-Mg alloy.

Key words: Al-Mg alloy; Zr; Sc; covalent bond; grain refinement; mechanical properties
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1 INTRODUCTION

The aluminum alloy containing minor Sc that has excellent performances, such as high toughness, and strength, good weld performance and corrosion resistance, were used widely in space flight, automobile and naval vessel as a new structural material. With the improvement of requirement to space flight and aviation material, modifying and developing of the aluminum alloys containing Sc and Zr on microstructure level have become the focal point that the material scientists paid close attention[1-4] to Al-Mg alloy at present.

In recent years quite a few international and domestic scholars[3-7] have systematically studied Al-Mg alloy containing minor Sc, Zr elements. The results show that, when different Sc contents are added, the effect of grain refinement of casting Al-Mg alloy is different apparently. Adding Sc(about 0.3%) improves the strength, hardness and other mechanical properties of casting Al-Mg and raises the thermal-stability of the alloy at the same time[8,9]. If Sc and Zr are added at the same time, the effect is more remarkable. It is suggested that the effect of minor Zr and Sc addition on the properties of alloy has an inherent relation to the strong interaction between Sc and Zr atoms and other atoms in matrix, especially in inner relation between bond characteristics of Sc, Zr and Al atoms.

Based on Pauling's valence theory [10] and the energy band theory, the empirical electronic theory in solid(EET)[11] has offered a simple, direct and practical experience method—BLD method to deal with valence electron structures of complicated system and has been used in segregation and design of alloys successfully[12,13]. Furthermore it enables to trace the macrophysics properties of the alloy back to its source on the valence electron structure level and offers theory guide in deep level in alloy design[14,15]. The purpose of this paper is to reveal the microcosmic mechanism of minor Sc and Zr addition to the property improvement of the casting Al-5%Mg alloys on the valence electron structure level from the bonding between the atoms.

2 MODEL OF CELL STRUCTURE

The α(Al) matrix is face-centered cubic structure to the Al-rich Al-Mg alloy. After the Mg atom is dissolved in Al matrix, Mg substitutes the positions of Al atoms, and forms Al-Mg solid solution. As pointed out in Ref.[15], when the content of Mg is not very high, Al-5%Mg solid solution is made up of

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two kinds of structure unit cells. One is the Al cell without Mg, the other is the Al cell containing Mg.

The lattice constant a_0 of Al crystal is 0.404 96 nm[16]. The lattice constant is increased by 0.000 5 nm when the addition of Mg is increased by 1%. The lattice constant of Al-Mg solid solution containing 5% Mg is 0.4074 5 nm, thus the lattice constant of the cell containing Mg is 0.416 32 nm[15].

When minor Sc or Zr is added singly or simultaneously in Al-Mg alloy, for the radii of Sc and Zr atoms are near to the radius of Mg atom, Sc atoms and Zr atoms substituted for Al atoms lie in the face center of Al cell. According to Ref. [12], besides pure Al and Al-Mg unit cell, Al-Mg-Sc-Zr solid solution alloy may include six kinds of unit cells such as Al-Zr, Al-Sc, Al-Sc-Zr, Al-Mg-Sc, Al-Mg-Zr and Al-Mg-Sc-Zr cells. The solid solution is composed of these six possible unit cells by mixing. The structure models of these cells are shown in Fig. 1 and Fig. 2. That Zr, Sc replace Al atom makes the lattice constant of Al-Mg-x cell change along with the change of x content, which will bring difficulty to use BLD analysis. Since the content of Zr, Sc in the alloy is little, the lattice constants of Al-Zr, Al-Sc cell can be replaced by that of pure Al cell and the lattice constants of Al-Mg-Zr, Al-Mg-Sc can be replaced by that of Al-Mg cell when such problem is handled. The impacts of Sc and Zr on lattice constant, i.e. the change of bond lengths caused by Sc, Zr substituting for Al atom, can be reflected by the change of atom-hybrid-state of Sc and Zr [12].

When minor Zr, Sc are added simultaneously, Al_3Sc and $Al_3(Zr_xSc_{1-x})$ composite phases which have $L1_2$ structure are precipitated in supersaturated solid solution. Besides Al-Mg, Al-Mg-Sc, Al-Mg-Zr and Al-Zr-Sc cells, the solid solution should include the particles of Al_3Sc, Al_3Zr and $Al_3(Sc, Zr)$ whose crystal structures are shown in Fig. 3. The lattice constants of Al_3Sc and Al_3Zr particles with $L1_2$ structure are 0.410 6 nm

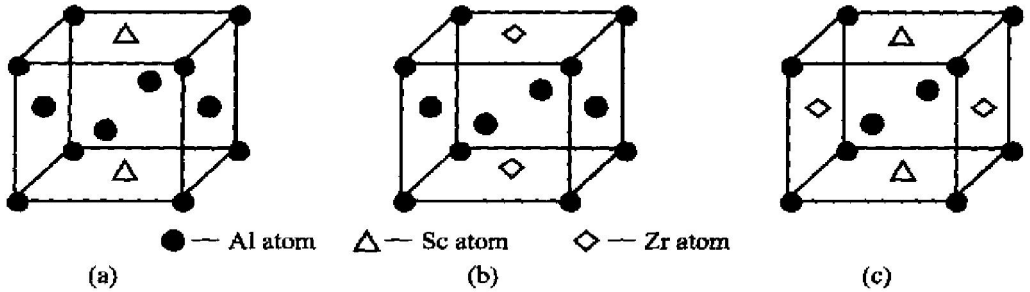

Fig. 1 Structural models of Al-Sc cell(a), Al-Zr cell(b) and Al-Zr-Sc cell(c)

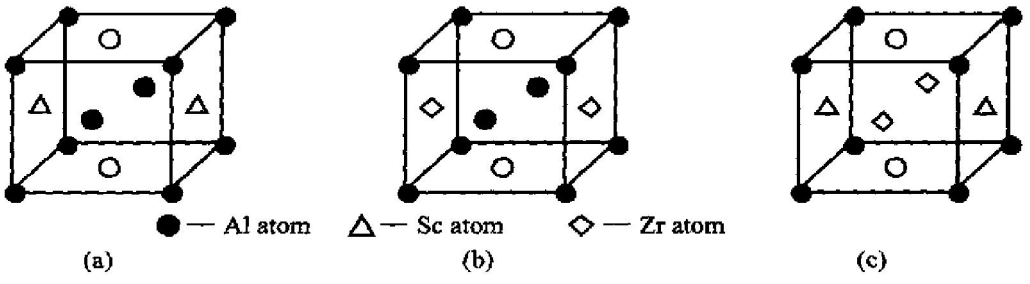

Fig. 2 Structural models of Al-Mg-Sc cell(a), Al-Mg-Zr cell(b) and Al-Mg-Sc-Zr cell(c)

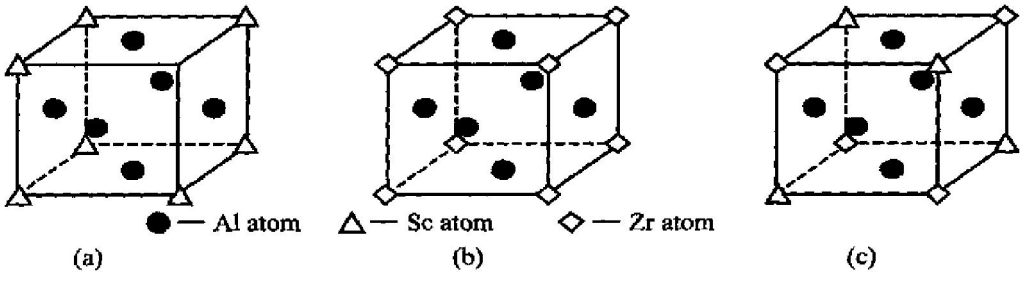

Fig. 3 Structural models of Al_3Sc(a), Al_3Zr(b) and $Al_3(Sc_{1-x}Zr_x)$(c)

and 0.405 nm[16] respectively. In $Al_3(Sc_{1-x}Zr_x)$ composite particle, Zr atom which may substitute for Sc in Al_3Sc phase is up to 50%[18]. The change of lattice constant because of Zr substituting for Sc can be reflected by the change of atom-hybrid-state of Zr atom.

3 CALCULATION METHOD AND RESULTS

According to EET[11], covalent electrons distribute in the bonds of the nearest neighbor, the second-nearest neighbor and sth neighbor. The amount of covalence electrons of every bond (namely bond order n_s) can be represented by the following bond length formula,

$$D(n_s) = R^u + R^v - \beta \lg n_s \quad (1)$$

where R is the radius of single bond, β is constant. The amount of covalence electron in a cell can be represented by the following equation:

$$k_1 n_c^u + k_2 n_c^v = \sum_s I_s n_s \quad (2)$$

The number of u, v atoms in the cell is represented by k_1, k_2 respectively. n_c^u, n_c^v are the amount of covalence electrons of u, v atoms respectively. I_s is the number of equivalence-bond of n_s. The equivalence-bond can be decided according to Ref. [11].

Based on the known crystal structure and lattice constant, the electronic structure of the cells can be calculated one by one with BLD-method[11] and BLD-criterion[11], through setting up n_A equation, combining Eqn. (1) and (2), and the detailed procedures are shown in the Refs. [11, 15, 19, 20]. The results of the strongest bond of every cell are shown in Tables 1, 2 and 3. The β is determined according to Eqn. (3-14) in Ref. [11].

Table 1 Valence electronic structures of Al, Al-Sc, Al-Mg, Al-Mg-Sc and Al_3Sc cells of Al-Mg-Sc alloy

Constitutional unit	Atomic hybridization state				Strongest covalent bond	n_A	ΔD_a/nm
	σ_{Al}	σ_{Mg}	σ_{Sc}	σ_{Zr}			
Al	4	–	–	–	Al—Al	0.208 6	0.000 7
Al-Mg	4	3	–	–	Al—Mg	0.203 6	0.000 5
Al-Sc	5	–	2	–	Al—Sc	0.252 6	0.002 9
Al-Mg-Sc	5	3	2	–	Mg—Sc	0.240 2	0.003 2
Al_3Sc	5	–	3		Al—Sc	0.263 1	0.000 3

Table 2 Valence electronic structures of Al, Al-Mg, Al-Zr, Al-Mg-Zr cells and Al_3Zr cell of Al-Mg-Zr alloy

Constitutional unit	Atomic hybridization state				Strongest covalent bond	n_A	ΔD_a/nm
	σ_{Al}	σ_{Mg}	σ_{Sc}	σ_{Zr}			
Al	4	–	–	–	Al—Al	0.208 6	0.000 7
Al-Mg	4	3	–	–	Al—Mg	0.203 6	0.000 5
Al-Zr	5	–	–	12	Al—Zr	0.304 1	0.000 3
Al-Mg-Zr	5	3	–	12	Mg—Zr	0.296 4	0.000 1
Al_3Zr	5	–	–	12	Al—Zr	0.306 1	0.000 3

Table 3 Valence electronic structures of Al, Al-Mg, Al-Sc-Zr, Al-Mg-Sc-Zr cells and $Al_3(Sc_{1-x}Zr_x)$ cell of Al-Mg-Zr-Sc alloy

Constitutional unit	Atomic hybridization state				Strongest covalent bond	n_A	ΔD_a/nm
	σ_{Al}	σ_{Mg}	σ_{Sc}	σ_{Zr}			
Al	4	–	–		Al—Al	0.208 6	0.000 7
Al-Mg	4	3	–	–	Al—Mg	0.203 6	0.000 5
Al-Sc-Zr	5	–	2	13	Sc—Zr	0.309 3	0.004 0
Al-Mg-Sc-Zr	5	3	2	13	Sc—Zr	0.240 3	0.003 8
$Al_3(Sc_{1-x}Zr_x)$	5	–	2	13	Al—Zr	0.322 8	0.000 6

4 ANALYSIS AND DISCUSSION

4.1 Effect of 0.2% and 0.5% Sc added separately in Al-Mg alloy

The Al—Sc bond is stronger than those of Al—Al and Al—Mg and the amount of valence electron of the strongest bond, namely the value of n_A was 0.263 1 in the casting Al-Mg-Sc melting alloy with Sc added singly, which can be known from the calculation result in Table 1. It is indicated that the coalescent incline of Al and Sc is strongest, and the covalent bond with p-d electron is easily formed. The Al-Sc phase diagram shows that the precipitated temperature of Al_3Sc in Al-Sc melting is 930 K which is much higher than the solidification temperature(830 K) of the Al-Mg alloy. Therefore, some Al atoms and Sc atoms are combined to form primary Al_3Sc particles before the Al-Mg alloy solidifies. The primary Al_3Sc particles with $L1_2$ crystal structure are coarser and coherent with matrix. The inhomogeneous nucleation is easily formed in Al-Mg alloy during solidification because interface energy between Al_3Sc and matrix is very low. The limited solid solubility[17] of Al-Sc is 0.2% Sc(mole fraction), and so, the number of primary Al_3Sc particles precipitated from the melting is very small when the percentage of Sc is less than 0.2%. In this case, the Sc atoms mainly exist in Al-Mg matrix in the form of solid solution, so the effect of grain refinement of Sc in Al-Mg alloy is not notable. On the contrary, when the content of Sc was more than 0.2%, because of the stronger combination inclination between Al and Sc, quite a lot of Sc atoms are firstly precipitated in the form of Al_3Sc, then grow up to coarse primary Al_3Sc particles in the melting. These great amount of Al_3Sc particles become the inhomogeneous nuclei of Al-Mg alloy during solidification, play a great role in grain refinement and improve the toughness of alloy. The experimental results of grain refinement in Refs. [5, 6] can be well explained in terms of the atom bonding.

The strongest covalent bond is the Al—Sc bond in Al-Sc cell whose amount of valence electron is n_A = 0.252 6, which is known from Table 1, in which the strongest covalent bonds of each segregation cell containing Sc are given. And the strongest covalent bond in Al-Mg-Sc cell is Mg—Sc bond whose amount of valence electron is n_A= 0.240 2. The above two strongest covalent bonds, Al—Sc bond and Mg—Sc bond, are much stronger than the strongest covalent bonds in Al cell without Mg and Al cell containing Mg. Therefore, Sc atom prior to combine with Al and enter the pure Al cell without Mg, not the Al cell with Mg. So in the view of the microstructure of solid solution, the Al cell containing Sc does not disperse in the form of single cell in the solid solution, but forms Al-Sc segregation region depended on the strong Al—Sc atom bond in the matrix.

Some Sc atoms precipitate as coarse primary Al_3Sc particles from the melting during solidification, the other Sc atoms exist mainly in the form of solid solution in the matrix of Al-Mg-Sc alloy. The saturate solubility of Sc decreases when the solidification temperature of the alloy declines, which makes the alloy become supersaturated Sc solid solution. In the following homogeneous treatment course, the tiny second Al_3Sc particles are easily precipitated homogeneously and dispersed in the Al-Sc segregation region. These tiny Al_3Sc particles are completely coherent with matrix and so their grain boundary has excellent lattice matching relation with matrix, then the Al—Sc covalent bond in tiny Al_3Sc particle improves the covalent bond of the matrix, plays a role in dispersion strengthening and improves the strength and hardness of the alloy. If these tiny Al_3Sc particles are precipitated in the grain boundary, because the crystal structure of Al_3Sc is the same as that of the matrix, they will strengthen the atom bond in the grain boundary, improve the bond strength of the grain boundary and play a role in sub-grain strengthening. Likewise, due to its high melting point and good thermal-stability, Al_3Sc particles which have strong Al—Sc covalent bond, benefit the stability of grain boundary, restrain the transfer of grain boundary under high temperature, hinder the recrystallization of the alloy, therefore keep the tiny grain and maintain excellent mechanical properties.

4.2 Effect of 0.2% Sc and 0.1% Zr added simultaneously in Al-Mg alloy

In Table 2, the strongest Al—Zr covalence bond, namely n_A of Al_3Zr cell, is n_A= 0.306 1 when Zr is added singly to the casting Al-Mg alloy. The strongest bond of Al—Zr atom in Al-Zr alloy is stronger than that of Al-Mg and Mg-Zr segregation cell, which shows that the combination tendency of Al and Zr atoms is the greatest and the covalent bond of p-d electron is easily formed. From the phase diagram of Al-Zr alloy, the precipitation temperature of Al_3Zr in the 0.17% Zr(mole fraction) solid solution is 1 250 K, which is higher than that of Al-5% Mg alloy, namely 830K. So there are quite a lot of Zr and Al atoms formed the primary Al_3Zr particles before Al-Mg-Zr alloy solidifies. The primary Al_3Zr particles crystallized in the solid solution, whose structure is the same as the face-centered cube structure of matrix with Ll_2 crystal structure, are relatively coarser. The Al—Zr bond in Al_3Zr is much stronger than Al—Sc bond in Al_3Sc. Therefore, under melting state the primary Al_3Zr particles are crystallized more easily than the primary Al_3Sc particles, and also the number of Al_3Zr particles is more than that of Al_3Sc particles,

namely the number of Al_3Zr as inhomogeneous nucleation is more than that of Al_3Sc, so the effect of Zr single-added is more notable than that of Sc single-added in grain refinement, which has been verified by the results of experimental results[5, 6].

From Tables 1 - 3, the Al—Zr bond in $Al_3(Sc_{1-x}Zr_x)$ is stronger than the Al—Zr bond in Al_3Zr and the Al—Sc bond in Al_3Sc when 0.2% Sc and 0.1% Zr are added simultaneously. It is indicated that the $Al_3(Sc_{1-x}Zr_x)$ particles are more easily formed than the particles of Al_3Zr and Al_3Sc in casting Al-Mg-Sc-Zr melt during solidification. Because some Sc atoms in Al_3Sc cell are replaced by Zr atoms, which reduces the misfit degree of spacing constant between Al_3Sc and matrix, the inhomogeneous nucleation is more easily formed in Al-Mg alloy. The effect of Sc and Zr added simultaneously is more notable than that of Sc or Zr added singly, so the plasticity of the former is better, which can be seen from the experimental results[5, 9]. On the other hand, because the Al—Zr bond in Al_3Zr is stronger than the Al—Sc bond in Al_3Sc, the core of $Al_3(Sc_{1-x}Zr_x)$ composite particle in the Al-Mg-Sc-Zr solid solution is the Zr-rich $Al_3(Sc_{1-x}Zr_x)$ and the outer cover of it is Sc-rich $Al_3(Sc_{1-x}Zr_x)$. It is well explained why double-structure of $Al_3(Sc_{1-x}Zr_x)$ is shaped in view of atom bonding.

In Table 3, the Sc—Zr bond is the strongest among the bonds n_A of Al-Sc, Al-Zr and Al-Sc-Zr in segregate cell in the following cooling and solidifying course of Al-Mg-Sc-Zr alloy, the value of n_A is 0.3093, therefore, Sc and Zr atoms exist mainly in the form of segregation cell in Al-Mg solid solution. Then in the following homogeneous treatment course, the tiny secondary $Al_3(Sc_{1-x}Zr_x)$ particles are easily precipitated from the Al-Sc-Zr segregated region in the matrix, and cohere with the matrix with low misfit degree. Due to the strong Al—Zr covalent bond of $Al_3(Sc_{1-x}Zr_x)$, the precipitation of $Al_3(Sc_{1-x}Zr_x)$ in matrix increases the strength of total covalent bond in matrix, so the strength and hardness of the alloy are improved. The precipitation of $Al_3(Sc_{1-x}Zr_x)$ in sub-grain boundary also increases the strength of covalent bond, pins dislocation, strengthens the grain boundary and improves the hardness of alloy. The strongest covalent bond n_A is the Al—Zr bond in $Al_3(Sc_{1-x}Zr_x)$ cell, $n_A = 0.3228$, which is stronger than that of Al_3Sc and Al_3Zr, so the thermal-stability of $Al_3(Sc_{1-x}Zr_x)$ is better than that of Al_3Sc and Al_3Zr under high temperature, and furthermore the $Al_3(Sc_{1-x}Zr_x)$ particles hindering the migrating of sub-grain boundary and restraining recrystallization of grain are most notable. This is the reason that the highest crystallization temperature is 773 K when Sc and Zr are added simultaneously[9], higher than 673 K(or 550K) when Sc(or Zr) is added singly in Al-Mg alloy, and that the super-plasticity of the Al-Mg-Sc-Zr alloy keeps best under high temperature when Sc and Zr are added simultaneously.

5 CONCLUSIONS

1) The casting Al-Mg alloy containing minor Sc and Zr in melting state under high temperature, is easy to form covalent bond of p-d electron because the Al—Sc bond and Al—Zr bond are much stronger. So primary Al_3Sc and relatively coarse $Al_3(Sc_{1-x}Zr_x)$ particles with $L1_2$ type are formed firstly when the alloy begins to solidify. They become inhomogeneous nucleus in the solidification of the matrix and play a great role in grain refinement of the alloy. Sc and Zr added simultaneously are more favorable to precipitate primary Al_3Sc and $Al_3(Sc_{1-x}Zr_x)$ particles, and so the effect of grain refinement is more notable and the plasticity of the alloy becomes better.

2) In solidification of the casting Al-Mg alloy containing minor Sc and Zr, some of Sc or Zr atoms precipitate from the solid solution in the form of Al_3Sc or Al_3Zr particles, the surplus of Sc or Zr atoms are still dissolved in the solid solution alloy. Because Al—Sc, Al—Zr and Sc—Zr bonds are relatively stronger, Al-Sc, Al-Zr and Al-Sc-Zr segregation regions are easier to be formed. With reduction of solidification temperature, the alloy becomes Sc and Zr super-saturation solid solution. During the following homogeneous treatment the tiny secondary Al_3Sc and $Al_3(Sc_{1-x}Zr_x)$ particles are precipitated in the alloy.

3) Because the secondary tiny Al_3Sc, Al_3Zr and $Al_3(Sc_{1-x}Zr_x)$ particles are coherent with the matrix have strong Al—Sc, Al—Zr, Sc—Zr covalent bonds, the intensity of total covalent bond in the alloy will be improved by the precipitation, and so the hardness and strength of the alloy are enhanced. If these tiny secondary particles precipitate in the sub-grain boundary, they can enable to strengthen the sub-grain boundary, improve thermal-stability of the sub-grain boundary, restrain the transfer of grain boundary and recrystallization of grain under high temperature, so the thermal-stability of alloy with $Al_3(Sc_{1-x}Zr_x)$ particles is the best in high temperature.

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