
Calculated Enthalpies of Al-B Group Element Alloys by Subregular Model

Liao Shuzhi¹, Zhang Bangwei^{2,*}

¹Key Laboratory of Low Dimensional Quantum Structures and Quantum Control of Ministry of Education, Department of Physics, Hunan Normal University, Changsha, China

²College of Physics, Hunan University, Changsha, China

Email address

zbw1212@126.com (Zhang Bangwei), liaosz@126.com (Liao Shuzhi)

*Corresponding author

Citation

Liao Shuzhi, Zhang Bangwei. Calculated Enthalpies of Al-B Group Element Alloys by Subregular Model. *International Journal of Modern Physics and Application*. Vol. 5, No. 3, 2018, pp. 27-34.

Received: March 14, 2018; Accepted: April 3, 2018; Published: May 16, 2018

Abstract: There were no systematically theoretical calculations of the mixing enthalpies for the Al-group B alloy systems from the first principle, from the famous Miedema's theory, or from other atomic theory in the literature. Such calculations for the 9 binary Al-group B metal alloy systems therefore are the first time taken place systematically by a subregular model. The results show that the agreement between the calculations and experimental data are pretty good and could be accepted from the theoretical or experimental points of view. It also can be concluded from the results and those in other papers by the authors that the subregular model could be using for calculating the mixing enthalpies for all of the 45 alloy systems combined with the 10 group B metals of Al, Zn, Cd, Ga, In, Tl, Sn, Pb, Sb and Bi.

Keywords: Binary Al-B Group Alloy, Mixing Enthalpy, Subregular Model

1. Introduction

Al based alloys containing group II B to V B metals have applied broadly to various industrial fields. This is because they possess superior properties when adding one or two metals of group IIB to VB into aluminum. For example, Aluminum-zinc alloys are used widely as materials for protective coatings (galvan, galvalume) of steel components exposed to corrosive environments [1]. The alloys based on the Al-Zn system have been widely studied because of their low density and good ability to be cast. The zinc addition makes their attractive mechanical properties such as high strength/weight ratio, high toughness and very high ductility to be used in many industries, such as the automotive, military or aerospace industry [2]. In a paper published in 2018 [3], study of Al-35Zn and Al-35Zn-0.5Sc alloys shows that the addition of 0.5 Sc promoted the grain refinement of the Al-35Zn alloys during solidification, heat treatment, and hot rolling. The damping capacity and mechanical properties of the Al-35Zn alloy were improved by the Sc addition and hot rolling. Compared with the commercial Al alloys, the rolled Al-35Zn-0.5Sc alloy with 90% reduction showed balanced

mechanical properties, including high strength and reasonable ductility. In addition, the Al-Zn system have attracted a lot of scientific attention as a classic example of an alloy system for the study of the spinodal decomposition [4]. Generally speaking, Al-alloys from monotectic binary systems such as Al-In, Al-Pb and Al-Bi have been identified as promising alternatives for the manufacture of wear-resistant components in the automotive industry, being capable to replace Cu-Sn-Pb conventional bearing materials [5-7]. Early in 1982, a United States patent 4,358,291 [8] declared that Ga-rich liquid Al-Ga alloys can be used for the purpose of splitting water to produce H₂. Later on, scientists discovered that bulk quantities of solid Al-Ga alloys also exhibited this same water-reactivity, and eventually disclosed in United States patent application 20080056986 in 2007 [9]. Moreover, Al-Sb and other III-V Group semiconductor alloys are widely used in infrared detectors and guidance systems and thermal imaging equipment. It is evidently that the applications of the Al-B group II-V metal alloys are very important and widely.

Just because the importance of these alloys, people paid

much attention to the extensive study and experimental measurement of their basically properties, especially for their mixing/formation enthalpies (denoted by ΔH for simplicity). In 1973, Hultgren et al. summarized near all of the measured ΔH data of 8 Al-B group alloy systems in his book [10] except of that for the Al-Tl system. Later on, such measurements in these alloy systems are continually performed. Therefore, we even can find that there are several groups of measured data in one alloy system, as shown in the Table 1 and Figure 1 obviously below.

However, there is a lack of theoretical calculations of the ΔH for such metal systems. It is well known that Miedema's group developed a famous thermodynamic theory for calculating ΔH of binary transition metal alloys [11–13]. However, they did not calculate ΔH for binary alloys containing only main group metal. Using the same Miedema's method and formulas, our group recently calculated ΔH for some of these alloy systems including the alkaline metal alloys, rare earth–Mg alloys, rare earth–Al alloys, noble metal–Al alloys, and rare earth–4d transition metal alloys [14–18]. Zhang Bangwei and Jesser [19] have proposed a modified Miedema model, calculating the formation energies for ternary alloy systems consisting of combinations of structural metals with all constituents being transition and/or simple metals. And we have proved in detail [20] that the modified Miedema model in a binary alloy system just is a simplified subregular model, and the Miedema model is a regular solution model, as pointed out by Miedema et al. themselves [12], especially the Eq. (3) in Ref. [12]. The mixing enthalpies of 9 binary Al-B group metal alloy systems are systematically calculated for the first time with the subregular model in present investigation.

2. Theoretical Model

From the so-called “macroscopic atom picture” [11–13], considering the interactions between i and j atoms in a binary alloy solution, Miedema et al. obtained finally a key equation of the enthalpy of solution of liquid i in liquid j at infinite dilution for a binary alloy:

$$\Delta H_{i \text{ in } j}^0 = \frac{2PV_i^{2/3}}{n_i^{-1/3} + n_j^{-1/3}} \left[-(\Delta\Phi^*)^2 + \frac{Q}{P}(\Delta n^{1/3})^2 - \frac{R}{P} \right] \quad (1)$$

where V , Φ^* , and $n^{1/3}$ are the parameters, P , Q and R are the constants determined by Miedema. $\Delta H_{i \text{ in } j}^0$ values are used from the calculations by Miedema et al. [13] After considering the composition in an alloy of the constituents, they obtained a formula of formation (or mixing) enthalpy ΔH of an alloy (equation (2.25) in Ref. [13]):

$$\Delta H = f_j^i \Delta H_{i \text{ in } j}^0 \quad (2)$$

where f_j^i is a parameter, which is that the degree to which an atomic cell of metal i is in contact with dissimilar atomic cell j on average.

We use the subregular model to the formation of binary

alloy system. In addition, we use the Miedema's Eq. (1) to describe the interaction between the components of an alloy. Therefore, the main equation for the formation/mixing enthalpy of a binary alloy for the subregular model derived in detail in [20] is

$$\Delta H_{i \text{ in } j} = X_i X_j (X_j \Delta H_{i \text{ in } j}^0 + X_i \Delta H_{j \text{ in } i}^0) \quad (3)$$

where X_i and X_j are the atomic fractions of species i and j , respectively.

It must point out that the equation for the ΔH of an alloy from Miedema model is similar to that of the regular solution model, and our model is similar to one of the subregular models. That is why we called our model for calculating ΔH of a binary alloy system as subregular model.

The above energy just is the chemical part resulting from the electron factors of the constituents, and is the main contribution to the energy. In addition, the structural and elastic contributions to the energy of an alloy should also be considered. The structural contribution accounts for the difference between the valences and the crystal structure of the solute and solvent. However, this is expected to have only a minor effect when comparing with the elastic energy contribution [21], so, this term will not be considered in the present calculations. The elastic effect is from the difference in atomic size of the constituents. This term is not considered in the Miedema model. Similar to Eq. (3), the elastic energy, i.e. the size-mismatch contribution to the formation enthalpy in a binary system ΔH_{ij}^e is:

$$\Delta H_{ij}^e = X_i X_j (X_j \Delta H_{i \text{ in } j}^e + X_i \Delta H_{j \text{ in } i}^e) \quad (4)$$

where $\Delta H_{i \text{ in } j}^e$ is the elastic energy per mole of solute metal.

The following equation from the classical theory of elasticity obtained by Friedel [22] is used in the calculation.

$$(\Delta H_{i \text{ in } j}^e)_F = \frac{24\pi B_i \mu_j R_i R_j (R_i - R_j)^2}{3B_i R_j + 4\mu_j R_i} \quad (5)$$

where B_i and κ_i is the bulk modulus and compressibility of the solute respectively, and μ_j is the shear modulus of the solvent. The values of B , μ and κ for elements have been tabulated by Gschneidner [23]. R_i and R_j are the radii for solute and solvent atoms which are represented by using the half of the measured interatomic distance of elements [24].

Use ΔH_M to indicate the formation energy only from the calculation with chemical part, i.e. just with equation (3), and ΔH_{MF} to express those from the calculation of chemical part from equation (3) and the elastic energy from equation (4) using Friedel formula (5). We will see below that only the elastic energy needs to be considered for the Al-Cd system, other 8 alloy systems just need to consider the term of ΔH_M . In addition, we use ΔH_{exp} to express the measured values of enthalpies.

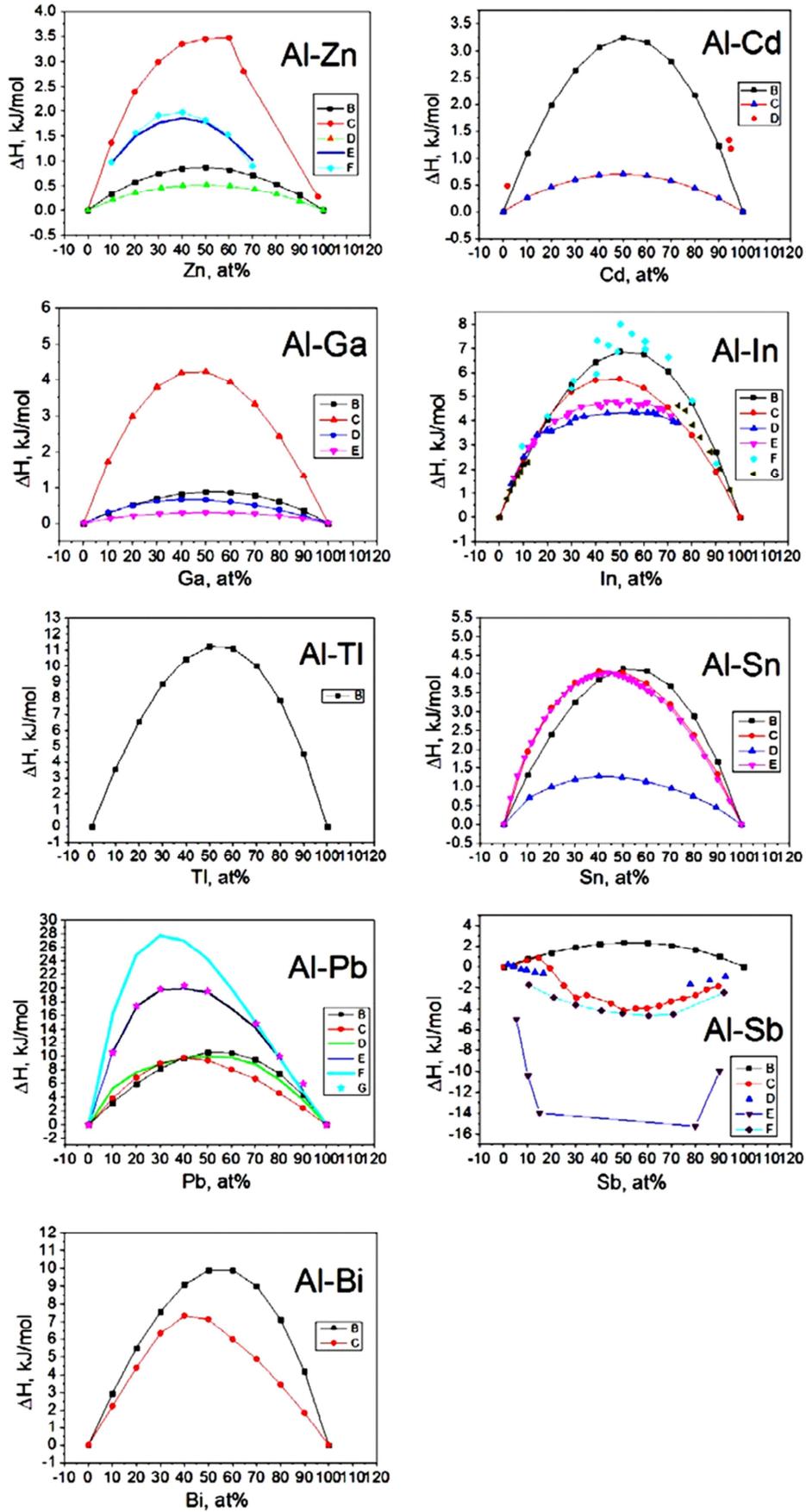


Figure 1. Calculated and experimental enthalpies of 9 binary Al-B group alloy systems. The symbols are indicated as in the Table 1.

3. Calculated Results

The calculated enthalpies for all of the 9 Al-B group metal alloy systems are shown in Figure 1. The calculating number of alloys in every alloy system is ten or more. In order to try to be simple and clear for the Figure, only one kind of the calculated data is presented on the figure, i.e. ΔH_M (■). This is because that the deviation between the calculations and experimental data increases when the elastic term is taken into account. However, there is only one exception for the alloy system Al-Cd because the agreement between the calculations and experimental data is improved when the elastic term is considered, so the values of ΔH_{MF} are used in the system. This

is similar with the calculations of the mixing enthalpies for 10 IIB-III B alloy systems [20], 11 IIB-IV B and IIB-V B alloy systems [25], theoretical Calculation of the Mixing Enthalpies of 21 III B-IV B, III B-V B and IV B-V B Binary Alloy Systems [26] and for various ternary alloy systems [19] via the subregular model.

Near all the experimental data for these alloys are presented on the figure. Up to date there is no any measured values of enthalpies in Al-Tl system can be found from literature, so only calculated values of enthalpies are presented. Table 1 lists all of cited sources including the measured temperature for measuring enthalpies.

Table 1. Detail captions of the Figure 1.

Alloy system	Theoretical calculation	Experimentals
Al-Zn	■ Subregular model. This work—First-principles calculation [27]	● Hultgren et al. [10], 1973, 653K
Al-Cd	■ Subregular model. This work ▲ Elastic contribution. This work	● Hultgren et al. [10], 1973, 950K
Al-Ga	■ Subregular model. This work ▲ Elastic contribution. This work	● Hultgren et al. [10], 1973, 1023K
Al-In	■ Subregular model. This work	● Hultgren et al. [10], 1973, 1173K
Al-Tl	■ Subregular model. This work	
Al-Sn	■ Subregular model. This work	● Hultgren et al. [10], 1973, 973K
Al-Pb	■ Subregular model. This work—D First-principles calculation [34]—E First-principles calculation [34]—F MAEAM calculation [35] ★ Miedema model cal. [35]	● Hultgren et al. [10], 1973, 1200K
Al-Sb	■ Subregular model. This work	● Yamaguchi et al. [36], 1995, 1350K
Al-Bi	■ Subregular model. This work	● Hultgren et al. [10], 1973, 1173K

From the Figure 1, several remarks can be drawn as below.

The agreement between the calculations and measured data is very good for the 6 alloy systems Al-Zn, Al-Cd, Al-Ga, Al-In, Al-Sn, and Al-Pb.

The agreement between the calculations and measured data is pretty good also when the contents of Bi are less than 50 at% for the Al-Bi system, but the deviation between the calculations and experimental data is rather large after the Bi contents are larger than 50 at%.

The problem is that in the Al-Sb system, the sign of the calculated mixing enthalpies is positive but most of the measured values are negative, which is just opposite. It should be said that this problem is not so serious because only one exception among the 9 Al-B group alloy systems. Such situation also existed in the calculations before [26] using the same subregular model. In fact, the situation that the sign of the calculated and measured enthalpies ΔH is just opposite is also appeared in the book by Miedema et al. [13]. For example, one can find that the calculated values of ΔH in Cr-Fe, Cr-Co and Cr-Ni systems are negative, but the measured ones are positive [p. 174 in 13]. In the Mn-Cr and Mn-Mo systems [p. 200 in Ref. 13] and in Co-Mg system [p. 272 in 13] the

calculated ΔH is positive, but the measured ones are negative. In the present subregular model, the values of $\Delta H_{i \text{ in } j}^0$ are the same as used by Miedema et al. in their calculations. Therefore one can easily deduce that this situation may come from the Miedema model. The Miedema model is very good, but is not completely perfect and still has possible flaw.

It can be seen from Figure 1 that the experimental scatter of calorimetric measurements for the same system usually is larger than or at least equal to the difference between calculations and measured values, which is especially obvious for 6 alloy systems Al-Zn, Al-Ga, Al-In, Al-Pb and Al-Sn. The calculated curves are all located among or closely near the measured curves in these 6 alloy systems.

In order to understand the calculations more deeply, considering the following two points would be helpful and useful.

First, the experimental data and the calculation results are more clearly compared. Putting the calculated results versus the experimental values of the maximum mixing enthalpies for the whole 9 Al-B group binary alloy systems (near 80 alloys) onto one figure, the deviations between them is illustrated very clearly, as shown in Figure 2. The fine solid line $y = x$

represents exact (100%) agreement between calculated and measured data, and the two outer thick lines indicate the defined data zone, with an error range of ± 2.0 kJ/mol. It is seen obviously that all the data are located within the area except few data points (about 5-6 alloys). Comparing a similar figure (Figure 2.31 in Ref. [13]) for the formation enthalpies in compounds of a transition metal (including the noble metals) and a polyvalent nontransition metal made by Miedema et al. themselves, it is easy to find that the consistency between the present calculations and experimental data of the mixing enthalpies for the whole 9 Al-B group binary alloy systems is somewhat superior to those from Miedema's original model

because the error range of the Figure 2.31 in Ref. [13] is ± 21 kJ/mol. Besides, the scatter in the Figure 2 of Ref. [40] for the formation enthalpies of the 260 intermetallic compounds calculated by the original Miedema model is worse than that in our Figure 2 because the error range in Figure 2 of Ref. [40] is ± 23 kJ/mol. Therefore, it can be concluded that the present calculations for ΔH of all 9 Al-B group metal systems are somewhat superior to those calculated by the original Miedema model for all transition alloy systems. It is believed that this advantage is the result of the difference between the subregular model and regular model.

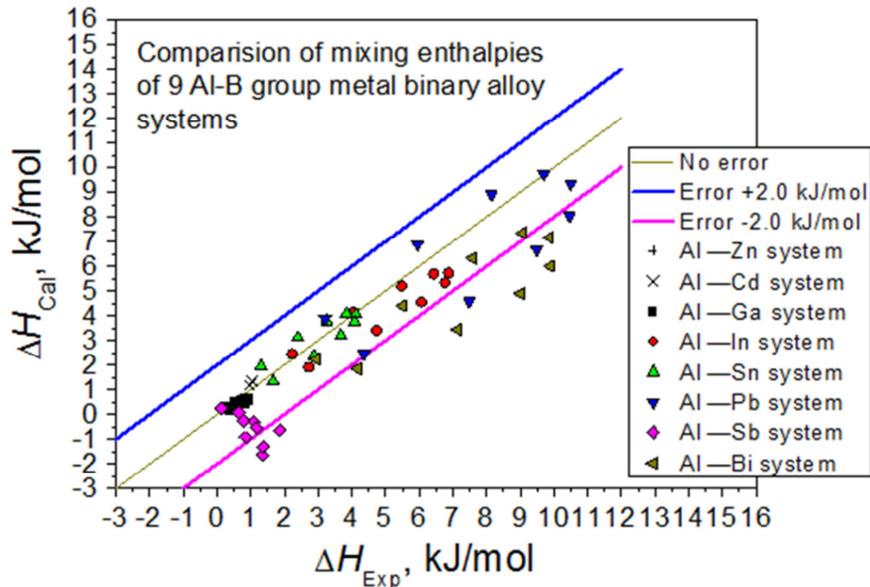


Figure 2. Comparison of calculations and experiment data of the mixing enthalpies for 9 Al-B group metal alloy systems.

Second, we calculated the errors between calculations and experiments for the 9 binary Al-B group alloy systems. As similar in the calculations for 11 IIB-IVB and IIB-VB binary alloy systems [25] and various ternary alloy systems [19], using $|\Delta H_{Exp}|$ and $|\Delta H_M|$ to present the average values of experimental data and of calculation results for all of the alloys of an alloy system, respectively, the error i.e. the ratio of average errors between calculations and measured data

$\frac{|\Delta H_{Exp} - \Delta H_M|}{|\Delta H_{Exp}|}$ for all of the alloys in every alloy system can be calculated, as shown in the Table 2. It can be seen from Table 2 that, the ratio is less than 20% for 4 alloy systems (Al-Zn, Al-Cd, Al-Sn and Al-In), and from 20% to 31.4% for other 3 systems (Al-Pb, Al-Bi and Al-Ga). Only one alloy system of Al-Sb, the ratio is rather large (73.91%). The results show that the errors between calculations and experiments for the 9 binary Al-B group alloy systems are pretty good except only one system (Al-Sb) is large.

Table 2. Calculated maximum mixing enthalpy, size factor and average errors of the present calculations compared to experimental data for the 9 binary Al-B group metal alloy systems, in kJ/mol.

Alloy system	Maximum enthalpy	Size factor, %	$ \Delta H_{Exp} $	$ \Delta H_{Exp} - \Delta H_M $	$\frac{ \Delta H_{Exp} - \Delta H_M }{ \Delta H_{Exp} }, \%$
Al-Tl	11.250	19.58			
Al-Pb	10.500	22.38	6.7213	1.5076	22.43
Al-Bi	9.888	8.39	7.9129	2.3960	30.28
Al-In	6.875	13.29	4.2640	0.8450	19.80
Al-Sn	4.125	8.39	3.0640	0.4260	13.90
Al-Cd	3.965	6.29	1.0050	0.1370	13.63
Al-Sb	2.375	1.40	0.5917	0.4373	73.91
Al-Ga	0.875	14.69	0.4913	0.1544	31.40
Al-Zn	0.869	4.19	0.3838	0.0171	4.50

These results indicate that the subregular model is suitable for the calculations of mixing enthalpies in the 9 Al-B group

binary alloy systems because the agreements between the calculations and measured values are good, which is the first

time for such systematic calculation in these alloy systems.

4. Discussions

In the following, the calculations will be discussed more deeply.

4.1. Effect of Atomic Size Factor on Mixing Enthalpies

Atomic size factor are very important parameters in the theory of alloy phases such as in the solid solubilities of alloys [41, 42]. Then, are there any effects of the size factor on mixing enthalpies for the 9 Al-B group metal alloy systems?

The expression $\frac{|R_i - R_j|}{\frac{1}{2}(R_i + R_j)}$ represents the size

factor of an alloy system, where R_i and R_j are the radii of solute and solvent atoms, that are a half of the measured interatomic distance of elements [24]. The calculated values of the size factor for every alloy systems versus ΔH are shown in Figure 3. Though there is a linear fit between the size factor and ΔH for five alloy systems Al-Cd, Al-In, Al-Sn, Al-Pb and Al-Sb, but the data are very scattered for other four systems Al-Zn, Al-Ga, Al-Tl and Al-Bi. In general it does not show any noticeable trend of the size effect on the ΔH in these 9 alloy systems. So, it may be concluded that the size factor is not the decisive or important factor for the magnitude of ΔH of 9 Al-B group alloy systems. This corresponds to the present calculating results, i.e., most of the alloy systems just need to use the ΔH_M to present ΔH , only one system need to consider the term ΔH_{MF} , which is including the elastic contribution caused by the size factor. Similar situation also appeared in the the 36 IIB to VB alloy systems [26].

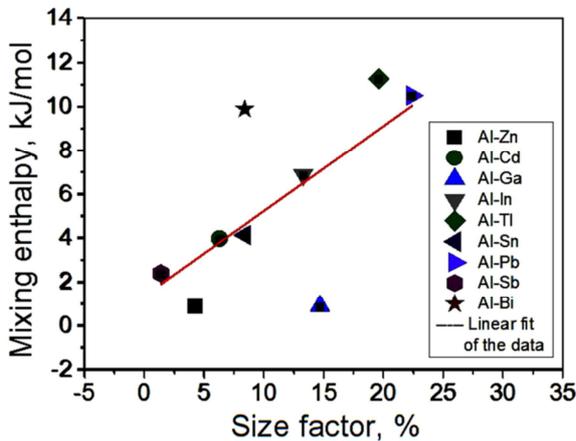


Figure 3. Relationship of the mixing enthalpies and size factor for the 9 binary Al-B metal alloy systems.

4.2. Relationship Between the Sign of ΔH and Phase Diagram

In Figure 4 an alloy system combined by Al and one of B group metals represents by either solid or dash line. The figure under each line is the calculated maximum mixing enthalpy for the alloy system, and the unit is kJ/mol. All of them are positive. However, the measured ΔH of Al-Sb is negative,

which is the only exception. Al and the 9 B group metals are all belongs to the polyvalent non-transition metal, their inner atomic shells (d and/or f) are all full with electrons, and only the out shells (s and/or p) have vacancies for electrons filling. That is to say from the point of view of atomic structure, all of the 10B group metals should not be very different but similar. However, when the alloys formed by Al with each B metal, the signs of mixing enthalpies are not all the same as mentioned above. How do we understand and explain such fact?

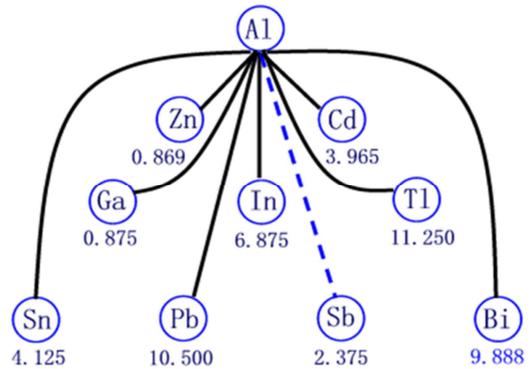


Figure 4. Relationship between the mixing enthalpies and the alloy phase diagrams for the 9 binary Al-B metal alloy systems. The figure is the maximum mixing enthalpy (in kJ/mol) of every alloy connected by the line of two metals.

The formation/mixing enthalpy of an alloy system depends on the interaction between atoms of constituents. Such interaction is very complicated, not only depending on the atomic structures of the constituents but also on the lattice structure, atomic size et al., therefore till today its picture is not very clear because of difficulty to illustrate or measure it. The positive mixing enthalpy means the reaction is endothermic during mixing a solution from constituents, indicating the instability of the alloy with respect to phase separation into its components. This situation occurs when the interaction between likewise atoms in the system is strong, but one between the unlike atoms is rather weak. On the contrary, the negative mixing enthalpy indicates the reaction is exothermic during mixing a solution from constituents, and the alloy/solution trends stability with respect to phase separation into its components. From the view point of alloy phase diagram, the former case indicates that the alloy phase diagram exists miscibility gaps in liquid phase or belongs to the so-called a pure eutectic type of phase diagram (type I phase diagram hereafter). And for the later case, the alloy phase diagram should exist one intermediate compound at least (type II phase diagram hereafter).

Figure 4 shows the details between the mixing enthalpies and phase diagrams for the 9 Al-B group alloy systems. The solid line indicates the alloy phase diagram of an alloy system formed by the two metals connected with the line is type I. And the dash line just indicates the type II phase diagram. It is obvious that only one alloy systems (Al-Sb) is exception, because its calculated ΔH is positive but its phase diagram is belonging to type II. The Al-Sb system exhibits a simple phase diagram with two eutectic points and an intermediate line

compound Al-Sb, so it belongs to type II. This exception obviously tells us that the sign of enthalpies does not depend completely on the type of phase diagrams, in other words, they do not exactly correspond though are closely related. The information of phase diagrams has been taken from [43]. It is interested to note that very recently some authors discussed the relationship between the sign of the formation enthalpy and the phase diagram for an alloy system, they used the similar view of points to explain their calculation results [44, 45].

4.3. Separating the Sign of Mixing Enthalpy with Miedema Coordinates

Miedema et al. used their model first for analyzing the signs of formation enthalpies for binary alloy systems, and have obtained a good separation between the positive and negative mixing enthalpies for the liquid equiatomic alloys of polyvalent non-transition metals by drawing a straightline with a very few exceptions (Figure 2.5 in Ref. [13]) using the values of Φ^* and $n^{1/3}$. Is there a similar good separation between the positive and negative mixing enthalpies for the 9 Al-B group metal alloys? Figure 5 shows the results. It can be seen that all of the calculated data of ΔH for the 9 alloy systems are located in their "correct" areas because their enthalpies are positive. However, the measured ΔH_{exp} of Al-Sb alloy system are all < 0 [36-39], indicating this system should be located in the "wrong" area ($\Delta H < 0$ area). Therefore, this once again shows that Miedema model has flaw. Of course, except Al-Sb system, the plot drawn by the two Miedema coordinates of $|\Delta\Phi^*|$ and $|\Delta n^{1/3}|$ can separate pretty good the signs of enthalpies for all the 8 Al- group B metal alloy systems.

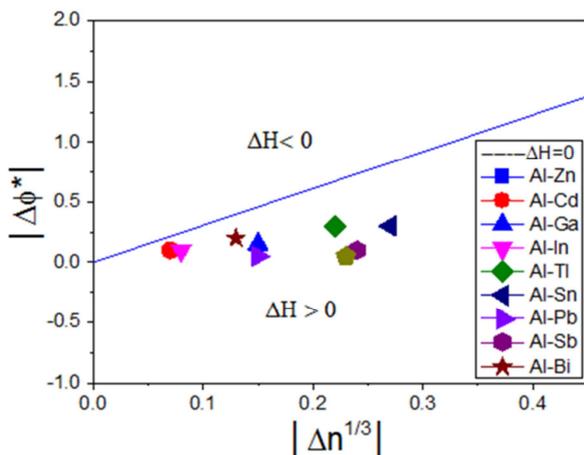


Figure 5. Separating enthalpies of the 9 binary Al-B group metal alloy systems.

5. Conclusions

Using the subregular model, the mixing enthalpies of 9 Al-B group binary alloy systems have been calculated first successfully, which have not been calculated systematically either by original Miedema model or by the theoretical methods from the first principle before.

The comparisons between the calculations and

experimental data of mixing enthalpies for the 9 alloy systems are good. General speaking, such comparison for the present results are some what superior to those from the original Miedema model of formation enthalpies calculations for transition metal alloys. The results prove that the subregular model can be used to calculate the mixing enthalpies for all of the binary alloy systems of B group metals.

The calculated maximum mixing enthalpies for these alloy systems do not exist obvious relationship with the size factor. That is why the mixing enthalpies are just only need the ΔH_M term of chemical attribution, and no need to add the elastic term for the 8 alloy systems but except only one system of Al-Cd.

Analysis indicates that the signs of enthalpies for the whole 9 Al-B group metal alloy systems are closely related on the type of phase diagrams though the Al-Sb system is the only exception.

The plot of the two Miedema's coordinates can separate the sign of the mixing enthalpies for the these alloy systems with only one exception for the alloy system of Al-Sb.

References

- [1] A. R. Marder, *Prog. Mater. Sci.* 45, 191 (2000).
- [2] A. Dębski, S. Terlicka, *J. Chem. Thermodynamics* 92, 91 (2016).
- [3] H. J. Jiang, C. Y. Liu, Y. Chen, Z. X. Yang, H. F. Huang, L. L. Wei, Y. B. Li, H. Q. Qi, *J. Alloys Comp.*, 739, 114 (2018).
- [4] J. Mainville, Y. S. Yang, K. R. Elder, M. Sutton, K. F. Ludwig, Jr. and G. B. Stephenson, *Phys. Rev. Lett.* 78 (14), 2787 (1997).
- [5] P. L. Schaffer, R. H. Mathiesen, L. Arnberg, *Acta. Mater.* 57, 2887 (2009).
- [6] E. S. Freitas, J. E. Spinelli, L. C. Casteletti, A. Garcia, *Tribol. Int.* 66, 182 (2013).
- [7] D. Mirkovic, J. Gröbner, R. Schmid-Fetzer, *Acta Mater.* 56, 5214 (2008).
- [8] J. J. Cuomo, J. M. Woodall, *Solid state renewable energy supply*, United States Patent 4, 358, 291, Nov 7, 1982.
- [9] J. M. Woodall, E. S. Harmon, K. C. Koehler, J. T. Ziebarth, C. R. Allen, Yuan Zheng, J.-H. Jeon, G. H. Goble, D. B. Salzman, *Power generation from solid aluminum*, United States Patent 7, 938, 879, Filed May 10, 2011.
- [10] R. Hultgren, P. D. Desai, D. T. Hawkins, M. Gleiser, K. K. Kelley, *Selected values of the thermodynamic properties of binary alloys* (Ohio, American Society of Metals 1973). P229 (Al-Zn); P137 (Al-Cd); P166 (Al-Ga); P173 (Al-In); P213 (Al-Sn); P196 (Al-Pb); P132 (Al-Bi).
- [11] A. R. Miedema, *J. Less Common Met.* 32, 117 (1973).
- [12] A. R. Miedema, P. F. de Chatel, F. R. de Boer, *Physica B+C* 100, 1 (1980).
- [13] F. R. de Boer, R. Boom, W. C. M. Mattens, A. R. Miedema and A. R. Niessen, *Cohesion in Metals, Transition Metal Alloys* (North-Holland, Amsterdam 1988).

- [14] Y. F. Ouyang, B. W. Zhang, S. Z. Liao, *Trans. Nonfer Metals Soc. China* 5, 94 (1995).
- [15] Y. F. Ouyang, B. W. Zhang, S. Z. Liao, Z. P. Jin, *Rare Metal Mater Eng.* 24, 24 (1995).
- [16] Y. F. Ouyang, B. W. Zhang, Z. P. Jin, S. Z. Liao, *Z. Metallkd.* 87, 802 (1996).
- [17] Y. F. Ouyang, S. Z. Liao, B. W. Zhang, Z. P. Jin, *Rare Metal Mater Eng.* 27, 142 (1998).
- [18] Y. F. Ouyang, Z. P. Jin, S. Z. Liao, B. W. Zhang, *Z. Metallkd.* 90, 242 (1999).
- [19] B. W. Zhang, W. A. Jesser, *Physica B*, 315, 123 (2002).
- [20] B. W. Zhang, S. Z. Liao, H. W. Xie, X. J. Yuan and X. L. Shu, *EPL: Lett. J. Explor Front Phys.* 89, 56002 (2010).
- [21] J. M. López, J. A. Alonso, L. J. Gallego, *Phys. Rev.* 36, 3716 (1987).
- [22] J. Friedel, *Adv. Phys.* 3, 446 (1954).
- [23] K. A. Gschneidner Jr, *Physical properties and inter-relationships of metallic and semimetallic elements. Solid State Phys.* 16, 275–426 (1964).
- [24] W. F. Gale, T. C. Totemeier, *Smithells Metals Reference Book*, 8th ed. (Oxford, Elsevier Butterworth-Heinemann, 2004).
- [25] B. W. Zhang, X. L. Shu, S. Z. Liao, X. J. Yuan and H. W. Xie, *J. Min. Metall. Sect B* 46, 141 (2010).
- [26] B. W. Zhang, S. Z. Liao, X. L. Shu, H. W. Xie and X. J. Yuan, *Phys. Metals Metallog.* 114 (6), 457 (2013).
- [27] S. Müller, L.-W. Wang, A. Zunger, *Phys. Rev. B*, 60 (24), 16448 (1999).
- [28] A. Yazawa, Y. K. Lee, *Mater. Trans. JIM* 11, 411 (1970).
- [29] S. an Mey, *Z. Metallkd.* 84, 451 (1993).
- [30] C. Girard, R. Baret, J. P. Bros, and P. Leydet, *J. Chim. Phys.* 74 (10), 1061 (1977).
- [31] B. Predel, H. Sandig, *Mater. Sci. Eng.* 4, 49 (1969).
- [32] R. N. Singhy, F. Sommer, *Rep. Prog. Phys.* 60, 57 (1997).
- [33] H. Flandorfer, M. Rechchach, A. Elmahfoudi, B. László, P. Arkadij, I. Herbert, *J. Chem. Thermodynamics* 43, 1612 (2011).
- [34] A. Landa, P. Wynblatt, D. J. Siegel, J. B. Adams, O. N. Mryasov, and X.-Y. Liu, *Acta Mater.* 48, 1753 (2000).
- [35] F. Fang, X. L. Shu, H. Q. Deng, W. Y. Hu and M. Zhu, *Mater. Sci. Eng. A355*, 357 (2003).
- [36] K. Yamaguchi M. Yoshizawa, Y. Takeda, K. Kamenda and K. Itagaki, *Mater. Trans. JIM* 36 (3), 432 (1995).
- [37] C. Girard, J. M. Miane, J. Riou, R. Baret and J. P. Bros, *J. Less Comm Met.* 128, 101 (1987).
- [38] T. J. Anderson, *The coupling of thermochemistry and phase diagrams for group III-V semiconductor systems*, Final Report. Prepared for the U.S. department of energy under grant number DE-FG05-86ER45276. July 21, 1998.
- [39] B. Predel, U. Schallner, *Mater. Sci. Eng.* 5 (4), 210 (1969/70).
- [40] R. F. Zhang, B. X. Liu, *Appl. Phys. Lett.* 81, 1219 (2002).
- [41] W. Hume-Rothery, G. W. Mabbott, and K. M. Channel-Evans, *Philos. Trans. R Soc. London, Ser A.* 233, 1 (1934).
- [42] B. W. Zhang, *Z. Metallkd.* 76, 264 (1985).
- [43] ASM Handbook Volume 03: Alloy Phase Diagrams, ASM International, 1992.
- [44] G. Vassilev, *J. Min. Metall.* 41, 79 (2005).
- [45] A. Yakoubi, L. Beldi, B. Bouhafis, M. Ferhat, *Physica B* 388 (1-2), 167 (2007).