

Original contributions

A simple analytical EAM model for bcc metals including Cr and its application

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Abstract. An analytical embedded atom method (EAM) model, which can treat bcc transition metal Chromium, has been developed. In this model, a new potential was presented, and a modified term has been introduced to fit the negative Cauchy pressure $P_c = (C_{12} - C_{44})/2$ for element Cr. The new model was applied to calculating the thermodynamic properties of binary alloys of all bcc transition metals V, Nb, Ta, Cr, Mo, W and Fe. The calculated dilute-solution enthalpies and formation enthalpies of random alloys are in good agreement with the experimental data available, the results from the first-principles calculations, and the results of thermodynamic calculations.

1. Introduction

Daw and Baskes [1] derived so-called EAM (embedded atom method) on the basis of quasiatom concept and density function theory. From then on, the semiempirical theory attracts great interest of scientists in materials science and condensed matter physics. It has been applied successfully to metals, impurity, surface, alloys, liquid and mechanical properties [1–13]. Johnson and Oh [14] proposed an analytical EAM model. This model was applied to calculating the thermodynamic properties for binary alloys of bcc transition metals V, Nb, Ta, Mo, W and Fe by Zhang and Ouyang [12], however, the model cannot treat transition metal chromium for its negative Cauchy pressure $P_c = (C_{12} - C_{44})/2$. Then, Pasianot, Farkes and Savino [15] proposed a so-called embedded defect potential, which can fit the negative pressure of chromium. At this point, the model of Pasianot et al. is successful, but the model, on one hand, has a complex expression, especially, the modified term did not be given clearly, on the other hand, the model has not any applications. So their model need testing extensively. Adams and Foiles [16] proposed an EAM model for metal vanadium, the model is not analytical.

In this paper, we present a new pair potential. In order to fit the negative Cauchy pressure, an analytic modified term $M(P)$ has been introduced. The developed analytical EAM model has been applied to calculating the self-diffusion properties of bcc transition metals [17]. The results are in excellent agreement with the available experimental values. So in this paper, the model was applied to calculating the dilute-solution enthalpies and formation enthalpies of binary alloys of bcc transition metals V, Nb, Ta, Cr, Mo, W and Fe.

2. Model

From the embedded atom method, the total energy of an assembly of atoms is [1]

$$E_t = \sum_i F_i(\rho_i) + \frac{1}{2} \sum_{\substack{i,j \\ i \neq j}} \phi(r_{ij}) \quad (1)$$

$$\rho_i = \sum_{j(\neq i)} f(r_{ij}) \quad (2)$$

where E_t is the total energy, ρ is the electron density at atom i due to all other atoms, $f(r_{ij})$ is the electron density distribution function of an atom, r_{ij} is the separation distance between atom i and atom j , $F(\rho_i)$ is the embedding energy to embed atom i in an electron density ρ_i , and $\Phi(r_{ij})$ is the two-body potential between atom i and atom j .

Following the previous procedure of EAM, the negative Cauchy pressure can not be fitted. So in the present model, an analytical modified term $M(P)$ has been introduced. Then (1) was written in the following form

$$E_t = \sum_i F_i(\rho_i) + \frac{1}{2} \sum_{\substack{i,j \\ i \neq j}} \Phi(r_{ij}) + \sum_i M(P_i) \quad (3)$$

$$P_i = \sum_{j(\neq i)} f^2(r_{ij}). \quad (4)$$

The introduction of the modified term $M(P)$ bases on two reasons. One is from (2), the total electron density in the position of atom i is the superposition of contribution from all other atoms. This assumption is too simple and neglects the hybridization and the polarity. The other is the spherical symmetric assumption of electron density distribution. In fact, the outer electron density distribution is not spherical symmetric except the S -electron. The modified term $M(P)$ represents the discrepancy between the assumption and the facts.

According to Johnson and Oh's procedure of development of EAM [14], the potential function satisfies the following equations

$$4\Phi(r_1) + 3\Phi(r_2) = -E_{1f} \quad (5)$$

$$4\Phi'(r_1) + 3\Phi'(r_2) = 0 \quad (6)$$

$$4\Phi''(r_1) + 3\Phi''(r_2) = 15\Omega G \quad (7)$$

$$\frac{8(r_1^2\Phi''(r_1) - r_1\Phi'(r_1))}{9(r_2^2\Phi''(r_2) - r_2\Phi'(r_2))} = A \quad (8)$$

The embedding function and the modified term satisfy the following equations

$$F(\rho_e) = -F_0 \quad (9)$$

$$F'(\rho_e) = 0 \quad (10)$$

$$F''(\rho_e) \frac{(8r_1f'(r_1) + 6r_2f'(r_2))^2}{(8f(r_1) + 6f(r_2))^2} \quad (11)$$

$$+ M''(P_e) \frac{4(8r_1f(r_1)f'(r_1) + 6r_2f(r_2)f'(r_2))^2}{(8f^2(r_1) + 6f^2(r_2))^2}$$

$$= 9\Omega B - 15\Omega G$$

$$M(P_e) = 0 \quad (12)$$

$$M'(P_e) = 0, \quad (13)$$

where E_{1f} is the monovacancy formation energy, r_1 and r_2 are the nearest- and next-nearest neighbor distances respectively, the prime indicates the differentiation to its argument. Ω is the equilibrium volume of an atom, G is the Voigt shear modulus, $G = (C_{11} - C_{12} + 3C_{44})/5$, C_{11} , C_{12} and C_{44} are elastic constants, A is the anisotropic ratio, $A = 2C_{44}/(C_{11} - C_{12})$, B is the bulk modulus, ρ_e is the equilibrium value of total electron density ρ , P_e is the equilibrium value of P , F_0 is the value of embedding function at equilibrium.

To get an applicable EAM model, the embedding function $F(\rho)$, the atomic electron density distribution function $f(r)$, the two-body potential $\Phi(r)$ and the modified term $M(P)$ must be determined. In this present model, the embedding function $F(\rho)$ is taken as the form of Johnson's general formula [14], namely

$$F(\rho) = -F_0 \left[1 - \ln \left(\frac{\rho}{\rho_e} \right)^n \right] \left(\frac{\rho}{\rho_e} \right) \quad (14)$$

where the parameters F_0 and n are determined as follows,

$$F_0 = E_c = E_{1f} \quad (15)$$

$$n = \sqrt{\frac{\Omega B}{A\beta^2 E_{1f}}} \quad (16)$$

where E_c is the cohesive energy, β is the decay power of the atomic electron density distribution function.

The electron density distribution function of an atom $f(r)$ is taken as Johnson's [14]

$$f(r) = f_e \left(\frac{r_1}{r} \right)^\beta \quad (17)$$

where the parameter f_e was determined in the present model as follows,

$$f_e = \left(\frac{E_c - E_{1f}}{\Omega} \right)^{(3/5)} \quad (18)$$

and the model parameter β is empirically taken as 6 for all seven bcc transition metals. Certainly, its exact values can be obtained by fitting (17) to the results of Clementi et al. [18].

The two-body potentials function $\Phi(r)$ is taken as

$$\Phi = K_0 + K_1 \left(\frac{r}{r_1} \right)^2 + K_2 \left(\frac{r}{r_1} \right)^4 + K_3 \left(\frac{r}{r_1} \right)^{12} \quad (19)$$

with

$$K_0 = -\frac{1}{7} E_{1f} - 15\Omega G \frac{10097924A + 12332488}{96(1238475A + 825650)} \quad (20)$$

$$K_1 = 15\Omega G \frac{1633023A - 811174}{96(1238475A + 825650)} \quad (21)$$

$$K_2 = 15\Omega G \frac{688128 - 137781A}{32(1238475A + 825650)} \quad (22)$$

$$K_3 = 15\Omega G \frac{1024(2A - 1)}{1238475A + 825650} \quad (23)$$

As for the modified term, considering the two assumptions mentioned above, the real host electron density should be

$$\rho_{rel} = \rho + \Delta\rho \quad (24)$$

where ρ is the electron density of host obtained by the two assumptions. $\Delta\rho$ is the deviation results from the assumption of spheric distribution of atomic electron density and the assumption of linear superposition of electron density. Instituting ρ_{rel} into (14), the energy change, which results from $\Delta\rho$, is

$$\Delta E(\Delta\rho) \propto -(\Delta\rho)^2 \quad (25)$$

Because $\Delta\rho$ is very small, then

$$\Delta E(\Delta\rho) \propto \text{Exp}[-(\Delta\rho)^2] \quad (26)$$

Table 1. The input physical parameters

	V	Nb	Ta	Cr	Mo	W	Fe
a (Å)	3.0399	3.3008	3.3026	2.8845	3.15	3.16475	2.86645 [21]
E_c (eV)	5.3	7.47	8.089	4.10	6.81	8.66	4.29 [22]
E_{1f} (eV)	2.10	2.75	2.950	1.80	3.10	3.95	1.79 [23–31]
Ω_B (eV)	13.62	18.857	21.733	11.936	25.656	30.630	12.255 [32]
Ω_G (eV)	4.17	4.409	7.961	8.688	12.290	15.829	6.555 [32]
A	0.791	0.514	1.559	0.714	0.762	1.001	2.462 [32]

Table 2. The model parameters determined from the input physical parameters

	V	Nb	Ta	Cr	Mo	W	Fe
K_0	0.444	0.764	0.007	1.464	1.836	1.538	− 0.349
K_1	− 1.395	− 2.030	− 1.176	− 3.164	− 4.241	− 4.213	− 0.299
K_2	0.628	0.872	0.641	1.405	1.899	1.978	0.277
K_3	0.021	0.001	0.094	0.033	0.056	0.118	0.102
f_e	0.412	0.448	0.471	0.371	0.422	0.483	0.395
F_0	3.200	4.720	5.139	2.300	3.710	4.710	2.500
n	0.477	0.608	0.362	0.508	0.549	0.464	0.278
α	0.117	0.141	0.180	− 0.154	0.022	0.006	0.017
β	6	6	6	6	6	6	6

Baskes et al. [19] proposed that the electron density change $\Delta\rho$ results from polarity could be expressed as

$$\Delta\rho \propto \sum_{j \neq i} f^2(r_{ij}) \quad (27)$$

From the above considerations and (12) and (13), let P represents the $\Delta\rho$ and P_e represents the average value of P , and then the modified term $M(P)$ is empirically taken as

$$M(P) = \alpha \left[\left(\frac{P}{P_e} - 1 \right)^2 \right] \exp \left[- \left(\frac{P}{P_e} - 1 \right)^2 \right] \quad (28)$$

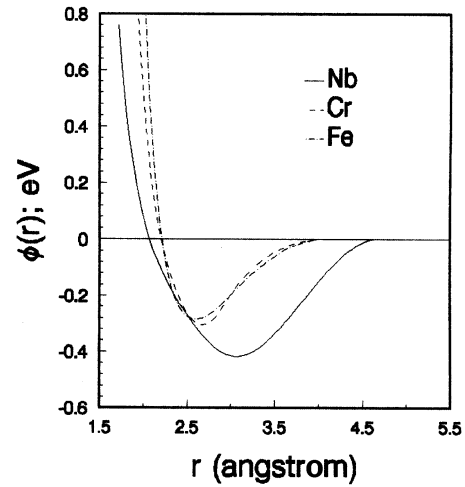
It has only one parameters α , which can be determined from (11) and (16).

Now the model parameters K_i ($i = 0, 1, 2, 3$), f_e , F_0 , n , α can be determined from the input physical parameters a , E_c , E_{1f} , B , G and A with the above equations, and only one adjustable parameter β is empirically taken as 6, so the present model is complete.

The input physical parameters are listed in Table 1, and the corresponding model parameters are listed in Table 2.

In the present model, the two-body potential and the electron density functions should be cut off. A cubic spline function is used as a cutoff function. The cutoff procedure is the same as that used by Zhang et al. [12] with the start point $r_s = r_2$, and the end point $r_c = \sqrt{2}r_2$.

Figure 1 shows the two-body potentials of Fe, Nb and Cr, and Fig. 2 shows the typical atom electron density function after cutoff. The present potential is similar to that of Johnson et al. [14] with stiffness within the

**Fig. 1.** The curves of two-body potentials for Nb, Cr and Fe

nearest-neighbor, and is better than that of Pasianot et al. [15], especially for Nb.

Figure 3 shows a typical embedding function, which is the same as that of Johnson et al. [14].

The comparison of the curve of total energy for the present model and Rose equation is shown in Fig. 4 for Fe and Cr. From the figure, it can be seen that the agreement between them is very good.

When the model is applied to studying the properties of alloy, the potential interaction between different type atoms must be defined. Here, the Johnson's [20] form

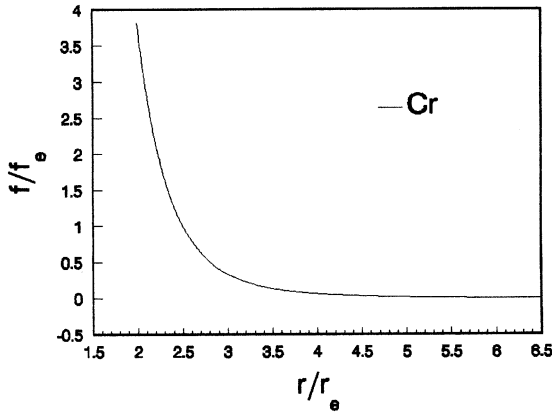


Fig. 2. A typical curve of atomic density distribution function

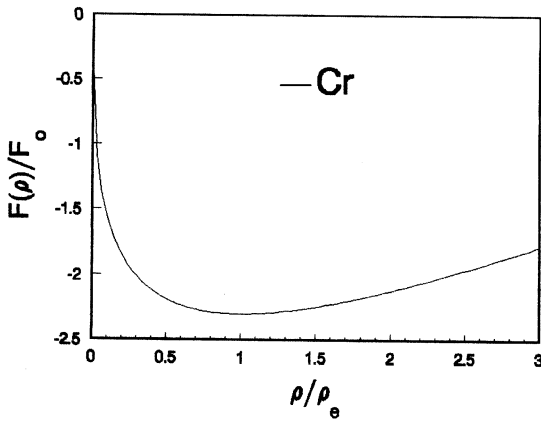


Fig. 3. A typical curve of embedding function

is taken,

$$\phi^{ab}(r) = \frac{1}{2} \left[\frac{f^a(r)}{f^b(r)} \Phi^{bb}(r) + \frac{f^b(r)}{f^a(r)} \Phi^{aa}(r) \right] \quad (29)$$

where a and b indicate the type of atoms.

3. Results and discussion

3.1. The dilute solution enthalpies

The present analytical EAM model is applied to calculating the dilute solution enthalpies of binary alloys of bcc metals V, Nb, Ta, Cr, Mo, W and Fe. The calculation procedure are similar to that described in details in [12]. The only differences is that there is an extra modified term in the equation of the total energy for the present model.

The comparison of the calculated dilute solution enthalpies to the available experimental data is shown in Fig. 5. From the figure, it can be seen that the calculated values are in good agreement with those of

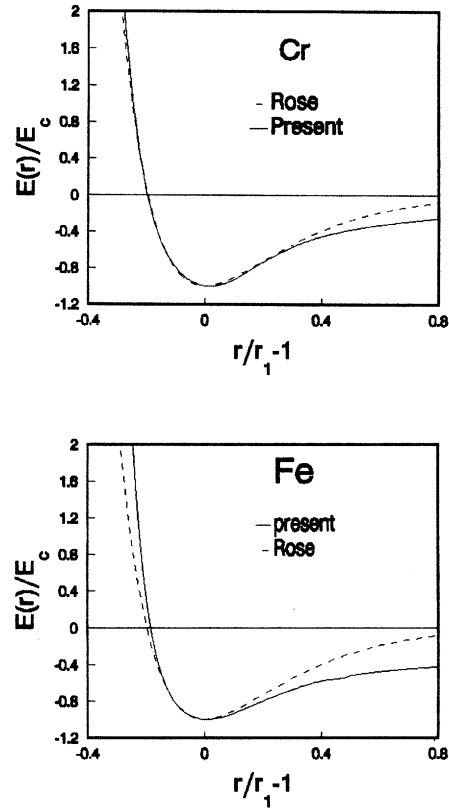


Fig. 4. The curves of total energy of present model (solid line) and the results of Rose's equation (dashed line) for Cr and Fe

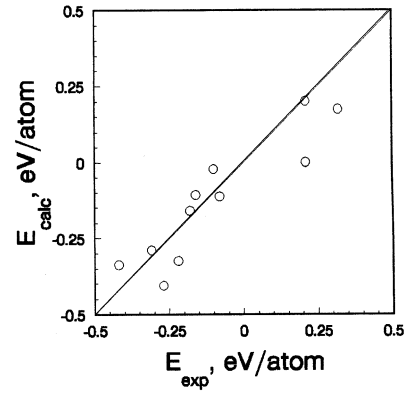


Fig. 5. The comparison of calculated dilute solution enthalpies with available experimental data. The diagonal line indicates exact agreement

available experiments. For Cr-Fe system, the present results deviate from the experiment's too more, but the sign or the trend is similar. For all W-bearing alloys, the present calculations are contrary to the results calculated with Johnson's model. Especially for Ta-W system, the present values are in excellent agreement with those of experiments, while the results of Johnson's model are contrary to those of experiments [12]. As to the rest of W-bearing alloys, experimental data cannot be found, so it is impossible to assert which are correct.

Table 3. The calculated dilute solution enthalpies and available experimental data, in eV/atom

Solvent	Solute						
	V	Nb	Ta	Cr	Mo	W	Fe
V		− 0.25	− 0.11	− 0.12 − 0.09 [33]	0.19	0.44	− 0.02 − 0.10 [34]
Nb	− 0.16		0.005	− 0.03	− 0.33 − 0.42 [35]	− 0.20	0.15
Ta	− 0.17	0.007		− 0.06	− 0.39	− 0.29 − 0.31 [36]	0.14
Cr	− 0.17 − 0.19 [33]	− 1.45	− 1.23		0.11 0.33 [33]	0.25	0.001 0.2 [33]
Mo	0.13	− 0.40 − 0.27 [35]	− 0.42	0.19 0.21 [33]		0.06	0.35
W	0.35	− 0.27	− 0.32 − 0.22 [36]	0.40	0.06		0.61
Fe	− 0.11 − 0.16 [34]	− 0.97	− 0.64	0.0001 0.22 [33]	0.31	0.60	

The correctness of results must be tested by experiments in the future.

In this paper, the dilute solution enthalpies for Cr-bearing alloys are calculated, which can not be calculated with Johnson’s model because the model can not describe the metal Cr. From the Table 3 and Fig. 5, we can see that the present calculated results are in good agreement with the available experimental data except the system Cr-Fe, for which the discrepancy between the calculations and experiments are much more.

For simplicity, the relaxation is not considered. The relaxation must affect the dilute solution enthalpy because of the difference of radius between solute and solvent atoms. This is the one of reasons caused the discrepancy between the calculation and experiment. The other reason may be the factor of temperature. The results of calculation are at 0K but the experimental data were obtained at nonzero temperature.

The complete comparison of calculated values to experimental data is impossible because of the limited experimental data. From the discussion above, we can see that the present calculations for dilute solution enthalpy are reasonably correct.

3.2. The formation enthalpies

The calculated formation enthalpies (solid curve) of the disorder alloys with any composition for 21 binary alloys of seven bcc transition metals are shown in Fig. 6. For comparison, the available experimental data (+), the ab initio calculations by Colinet et al. [37] (▲), the results of Spencer et al. [38] (△), the results of Sigli et al. [39] (■) and the results of the thermodynamic calculations by Miedema et al. [40–41] (····) are also shown in Fig. 6.

The results of Mo-Nb, Mo-Ta and Ta-W systems are in excellent with the available experimental data and the calculated values of Colinet et al., of Sigli et al. and of Miedema et al. respectively. The phase diagrams for the three alloy systems are all series solid solution and the structure of alloy in whole composition range is bcc,

which is consistent with our assumption. On the other hand, the percentages of the proportion of the discrepancy of lattice constant of two alloy constituents to the lattice constant $\Delta a/a\%$ for these systems are less than 5%, then the elastic distortion energies are very small and result in little influence on alloying. The excellent agreement are expected. Especially for the Ta-W system, the formation enthalpies from Johnson’s model is positive, while the experimental data are negative. The coincidence of the present results and the experimental data indicates that the present model is successful for Ta-W system.

The calculated results for Fe-V system are in reasonable agreement with available experimental data [34] and with the results of Spencer [38], especially, the asymmetry of the formation enthalpy is in excellent agreement with the results of experiments. The magnitude of present results is smaller than the results of experimental results. However, the values calculated with Miedema’s theory are larger than experimental data in magnitude. For experimental data, the results from different workers are different. In this paper, we use the results of Kubaschewski et al. [34] because both of the reference state of element and structure of alloy are bcc in Kubaschewski et al’s experiment, which is consistent with our assumption. The percentage of $\Delta a/a\%$ for Fe-V system is less than 6%, but the phase diagram of this system is not series solid solution in whole composition range at low temperature. The existence of σ phase makes the bcc structure assumption in the whole composition range for the present calculations deviated from the fact. On the other hand, the present calculation without dependence on temperature may be considered as the results of room temperature, while, the experimental data were measured at 1665 K. The factors mentioned above result in the discrepancy.

Chromium-bearing systems include Cr-Mo, Cr-V, Cr-Fe, Cr-Nb, Cr-W and Cr-Ta. From the phase diagrams of the six systems, Cr-V and Cr-Mo are series solid solution, and $\Delta a/a\%$ of two components for the two systems are less than 10%. The present calculations are in excellent agreement with those of experiments. For Cr-V system, the results of Miedema et al. are consistent with the present

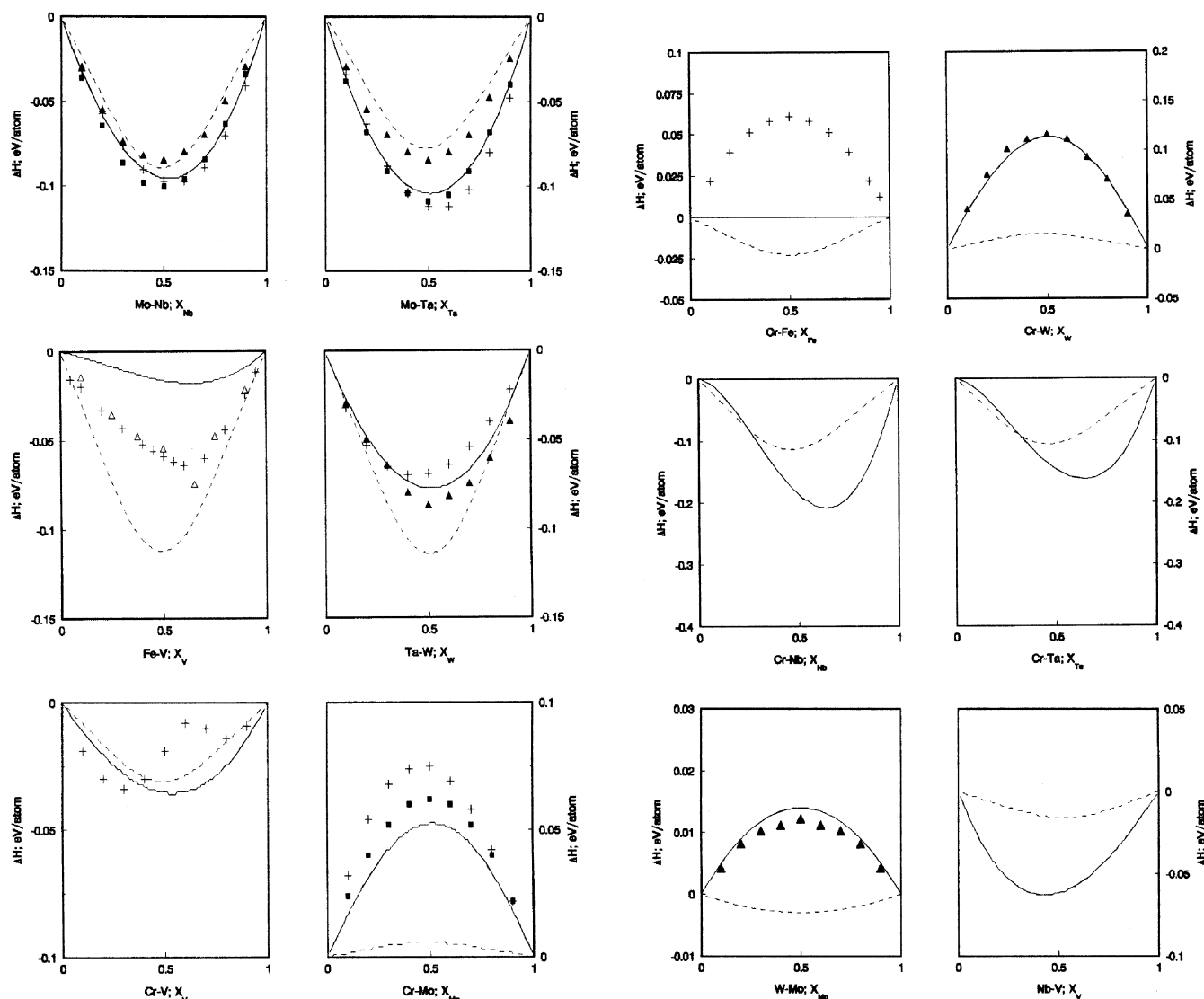


Fig. 6. The calculated formation enthalpies of random alloys in whole composition range. The present results (—), the results of first-principles calculations (\triangle Spencer, \blacktriangle Colinet, \blacksquare Sigli), the available experimental data (+) and the results of Miedema theory (---)

calculations. As to Cr-Mo system, the calculation of Colinet et al. is similar to the present results, both of them are larger than that of Miedema et al. in magnitude. Of the six systems, Cr-Fe and Cr-W have similar complexity in phase diagrams. The present calculations and those of Miedema et al. for Cr-Fe system indicate that the formation enthalpies are very small and both of them are less than the experimental data, the deviation of Cr-Fe system from experimental data may be result from existence of σ phase as discussed in Fe-V system. For Cr-W system, no experimental data have been found. The present results are in excellent agreement with those of Colinet et al. and both of them are much larger than those of Miedema et al. For Cr-Ta and Cr-Nb systems, the formation enthalpies are in good agreement with those of Miedema et al. From Fig. 6, it can be seen that the curve of formation enthalpy is not symmetric and the summit is close to Cr. The phase diagrams of the two systems

indicate that the solid solubilities of Nb and Ta in Cr is larger than those of Cr in Nb and Ta. The behavior of formation enthalpy can be easily explained by the fact.

For the Mo-W system, the present results are in good agreement with those of Colinet et al. and are much larger than those of Miedema et al. From the phase diagram of Mo-W system, we can see that it is series solid solution, then the agreement is easily understood.

For V-Mo, V-Nb, V-Ta and V-W systems, the formation enthalpies are in agreement with those of Miedema et al. except V-W, for which the sign of the present results is positive while that of Miedema et al. is negative. From the phase diagrams of these systems, they are all series solid solution except V-Ta, in which there is some complex situation in some composition range at low temperature. Because there are no experimental data available, further comparison can not be performed.

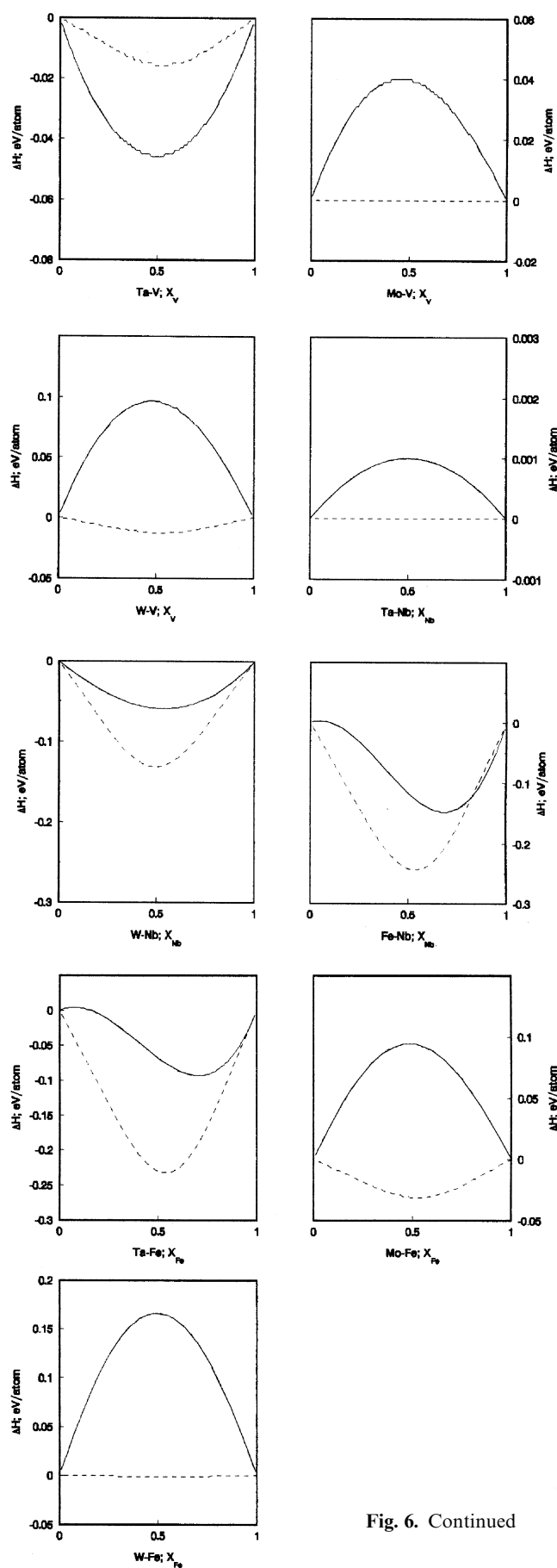


Fig. 6. Continued

For Nb-Ta and Nb-W systems, the calculated formation enthalpies are in agreement with those of Miedema et al. The two systems have very simple phase diagrams. It is interesting to note that the signs of formation enthalpy for the two systems are contrary, though they have similar phase diagrams. The formation enthalpies of Nb-Ta are very small, and those of Nb-W system are relatively large. As the lattice constants of Ta and Nb are nearly same, the distortion and the elastic energy are negligible, which may result in small formation enthalpies of Nb-Ta system. The mismatch Nb and W lattices is relatively large. The formation enthalpy may be considered resulting from the elastic mismatch energy.

As to the systems Nb-Fe, Ta-Fe, Mo-Fe and W-Fe, the present results of Nb-Fe and Ta-Fe are in good agreement with the results of Miedema et al. But for W-Fe system, the present calculations are much larger than those of Miedema et al. For Mo-Fe, the present results are positive while those of Miedema et al. are negative. The four alloy systems have complex phase diagrams. The lattice mismatch is large for the four systems. Whether the present calculations are correct or not, it has yet to be proved by further experimental works.

From the above discussions, we can see that the present results are in good agreement with those of experiments or the ab initio calculations or thermodynamic calculations. We may conclude that the present analytical EAM is successful in the calculations of thermodynamic properties for all of the transition bcc metals including Cr.

4. Conclusions

A simple analytical embedded atom method model for bcc metals including Cr has been developed. In the new model, a modified term of energy was introduced to fit the negative Cauchy pressure of Cr, and a new form of two-body potential was also proposed. This potential function can represent the interaction between atoms in the wide range. The introduction of new modified term overcomes the difficult that the EAM model can not treat metal Cr. All parameters of the model have been determined.

The calculated dilute solution enthalpies are in good agreement with the available experimental data.

The formation enthalpies are in good agreement with the available experimental data and those of the first-principles calculations. In the whole, the present results are generally good agreement with those calculated with Miedema's theory.

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