THEORY OF THE ORDER-DISORDER TRANSITIONS IN THE HEUSLER ALLOYS. IV

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The Machlin pair potential model was applied to estimate the interaction energy of atoms in the Heusler alloys $Cu_{3-x}Mn_xAl$ $(0 \leqslant x \leqslant 1)$ and $Cu_2Mn_{2-y}Al_y$ $(0 \leqslant y \leqslant 1)$. The phase diagrams of these alloys were calculated in the approximation of the interaction of atoms in two zone co-ordinations and they were compared with the experimental results of Bouchard and Thomas. The approximation used is discussed in the appendix.

1. Introduction

In the first part of the cycle of our papers [1] the theory of "order-disorder" transitions in the stoichiometrical Heusler alloys B_2AC was presented. The Bragg–Williams approximation was used and the interaction of pairs of atoms in one zone co-ordinations was taken into considerations. In subsequent papers [2, 3] a similar method was applied to the generalization of the theory to non-stoichiometrical alloys. The interactions of atoms in two zones co-ordinations were considered. Two particular cases were discussed:

a) where the number of atoms in an alloy is equal to the number of lattice points in a crystal, and

b) where the number of atoms is less than the number of lattice points in the crystalline lattice. This assumption is followed by the presence of "structural vacancies" in a crystal.

In the present paper the estimation of the interaction energies of the pairs of atoms in the Heusler alloys is presented. The estimated values of the energies were substituted into formulae (14) from paper [2]. With the aid of those formulae the critical temperatures of the "order-disorder" transitions in the alloys $Cu_{3-x}Mn_xAl$ and $Cu_2Mn_{2-y}Al_y$ were found. The applied approximation is analyzed in the appendix.

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2. The temperatures of the "order-disorder" transitions in the alloys $B_{3-x}A_xC$ and $B_2A_{2-y}C_y$

In order to simplify the considerations and to obtain a clear representation of the phase diagrams of the non-stoichiometrical Heusler alloys $B_zA_xC_y$, the concentration of atoms of only one component is introduced as an independent variable. The considered alloys are of the composition: $B_{3-x}A_xC$ and $B_2A_{2-y}C_y$.

In agreement with the considerations presented in our previous paper the process of the ordering of atoms in the Heusler alloys may be schematically represented as

$$A2 \xrightarrow{T_1} B2 \xrightarrow{T_2} L2_1,$$

another possibility is

$$A2 \xrightarrow{T_1^*} L2_1,$$
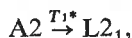
where T_1, T_2, T_1^* denote the critical temperatures of the "order-disorder" transitions and A2, B2, L2$_1$ are the symbols for the types of structures appearing in the Heusler alloys. The above critical temperatures may be calculated with the aid of Eqs (14) from paper [2] applied to the discussed composition of the alloys. Thus, they are given by the following formulae:

a) the alloys $B_{3-x}A_xC$

$$T_1 = \frac{1}{16k} \{x(3-x)\left[4W_{12}(r_1)-3W_{12}(r_2)\right]+(3-x)\left[4W_{23}(r_1)\right.$$

$$\left.-3W_{23}(r_2)\right]+x[4W_{13}(r_1)-3W_{13}(r_2)]+\sqrt{\Delta^*}\},$$

$$\Delta^* = \{x(3-x)\left[4W_{12}(r_1)-3W_{12}(r_2)\right]+(3-x)\left[4W_{23}(r_1)\right.$$

$$\left.-3W_{23}(r_2)\right]+x[4W_{13}(r_1)-3W_{13}(r_2)]\}^2-4x(3-x)$$

$$\times\{4[4W_{12}(r_1)-3W_{12}(r_2)][4W_{23}(r_1)-3W_{23}(r_2)]\}$$

$$+4x(3-x)\{4[W_{12}(r_1)+W_{23}(r_1)-W_{13}(r_1)]$$

$$-3[W_{12}(r_2)+W_{23}(r_2)-W_{13}(r_2)]\}^2,$$

$$T_2 = \frac{3}{16k}\{(x+S_{20})(1+S_{40})[2W_{13}(r_2)-W_{12}(r_2)-W_{23}(r_2)]$$

$$+(x+S_{20})(3-x-S_{20}-S_{40})W_{12}(r_2)+(1+S_{40})(3$$

$$-x-S_{20}-S_{40})W_{23}(r_2)+\sqrt{\Delta^*}\},$$

$$\Delta^* = \{(x+S_{20})(1+S_{40})[2W_{13}(r_2)-W_{12}(r_2)-W_{23}(r_2)]$$

$$+(x+S_{20})(3-x-S_{20}-S_{40})W_{12}(r_2)+(1+S_{40})(3$$

$$-x-S_{20}-S_{40})W_{23}(r_2)\}^2-16(1+S_{40})(x+S_{20})(3$$

$$-x-S_{20}-S_{40})\{W_{12}(r_2)W_{23}(r_2)-[W_{12}(r_2)+W_{23}(r_2)-W_{13}(r_2)]^2\},$$

$$T_1^* = \frac{3}{4k} \{[\tfrac{1}{4} x^2 W_{12}(r_2) + \tfrac{1}{4} x W_{23}(r_2) + \tfrac{1}{2} x W_{13}(r_2)] + \sqrt{\Delta^*}\},$$

$$\Delta^* = \left[\frac{x^2}{4} W_{12}(r_2) + \frac{x}{4} W_{23}(r_2) + \frac{x}{2} W_{13}(r_2)\right]^2$$

$$- 2x\{W_{12}(r_2)W_{23}(r_2) - [W_{12}(r_2) + W_{23}(r_2) - W_{13}(r_2)]^2\}. \tag{1}$$

b) The alloys $B_2 A_{2-y} C_y$

$$T_1 = \frac{1}{4k} \{(1 - \tfrac{1}{2} y)[4W_{12}(r_1) - 3W_{12}(r_2)] + \tfrac{1}{2} y[4W_{23}(r_1)$$

$$- 3W_{23}(r_2)] + \tfrac{1}{2} y(1 - \tfrac{1}{2} y)[4W_{13}(r_1) - 3W_{13}(r_2)] + \sqrt{\Delta^*}\},$$

$$\Delta^* = \{(1 - \tfrac{1}{2} y)[4W_{12}(r_1) - 3W_{12}(r_2)] + \tfrac{1}{2} y[4W_{23}(r_1)$$

$$- 3W_{23}(r_2)] + \tfrac{1}{2} y(1 - \tfrac{1}{2} y)[4W_{13}(r_1) - 3W_{13}(r_2)]\}^2$$

$$- y(1 - \tfrac{1}{2} y)\{4[4W_{12}(r_1) - 3W_{12}(r_2)][4W_{23}(r_1)$$

$$- 3W_{23}(r_2)]\} + y(1 - \tfrac{1}{2} y)\{4[W_{12}(r_1) + W_{23}(r_1)$$

$$- W_{13}(r_1)] - 3[W_{12}(r_2) + W_{23}(r_2) - W_{13}(r_2)]\}^2,$$

$$T_2 = \frac{3}{16k} \{(2 - y + S_{20})(y + S_{40})[2W_{13}(r_2) - W_{23}(r_2) - W_{12}(r_2)]$$

$$+ (2 - y + S_{20})(2 - S_{20} - S_{40})W_{12}(r_2) + (y + S_{40})(2$$

$$- S_{20} - S_{40})W_{23}(r_2) + \sqrt{\Delta^*}\},$$

$$\Delta^* = \{(2 - y + S_{20})(y + S_{40})[2W_{13}(r_2) - W_{23}(r_2) - W_{12}(r_2)]$$

$$+ (2 - y + S_{20})(2 - S_{20} - S_{40})W_{12}(r_2) + (y + S_{40})(2$$

$$- S_{20} - S_{40})W_{23}(r_2)\}^2 - 16(y + S_{40})(2 + S_{20} - y)(2$$

$$- S_{20} - S_{40})\{W_{12}(r_2)W_{23}(r_2) - [W_{12}(r_2) + W_{23}(r_2) - W_{13}(r_2)]^2\},$$

$$T_1^* = \frac{3}{4k} \left\{\left[\left(\frac{y}{2} - 1\right)^2 W_{12}(r_2) + \tfrac{1}{4} y^2 W_{23}(r_2) + y\left(1 - \frac{y}{2}\right) W_{13}(r_2)\right] + \sqrt{\Delta^*}\right\},$$

$$\Delta^* = \left[(1 - \tfrac{1}{2} y)^2 W_{12}(r_2) + \frac{y^2}{4} W_{23}(r_2) + y\left(1 - \frac{y}{2}\right) W_{13}(r_2)\right]^2$$

$$- 16\left(1 - \frac{y}{2}\right)\{W_{12}(r_2)W_{23}(r_2) - [W_{12}(r_2) + W_{23}(r_2) - W_{13}(r_2)]^2\}. \tag{2}$$

In the above formulae $W_{ik}(r_s) = 2V_{ik}(r_s) - V_{ii}(r_s) - V_{kk}(r_s)$ and $V_{ik}(r_s)$ denotes the interaction energy of a pair of atoms "i" and "k" separated by the distance r_s (the radius of the s-th zone co-ordinations). S_{20} and S_{40} denote the values of the long-range order parameters S_2 and S_4 at the temperature T_2.

The estimation of the parameters $W_{ik}(r_s)$ is necessary for the evaluation of the critical temperatures of the phase transitions.

3. A model of a pair interaction potential in an intermetallic phase

There are several conditions which must be fulfilled by the interaction potential $V_{ik}(r)$ of two atoms in a crystal which is in a stable state. They are:

1) The interatomic force $-\dfrac{\partial V_{ik}}{\partial r}$ must be attractive for great distances between atoms and must be repulsive for small distances. Thus the function $V_{ik}(r)$ must have a minimum at $r = r_0$.
2) When r increases, $V_{ik}(r)$ must decrease faster than r^{-3}.
3) All the elastic constants must be positive.
4) $C_{11} - C_{12} > 0$, where C_{11} and C_{12} are the elastic constants.

The conditions 1) and 2) follow the following simple considerations. The first is a condition for the appearance of condensed matter, the second arises from the assumption about the finite value of the cohesive energy of a crystal. Fulfilment of the remaining conditions assures stability with respect to infinitesimal strains. The analysis of the stability of a crystal and the derivation of the conditions 3) and 4) had been presented by Born [4].

In further considerations the well-known interatomic potential will be applied

$$V_{ik}(r) = -\frac{A_{ik}}{r^m} + \frac{B_{ik}}{r^n}, \tag{3}$$

where A_{ik} and B_{ik} are the parameters of attraction and repulsion depending on the interacting atoms. Machlin [6] introduced the above potential for the calculations of lattice parameters of some intermetallic solid solutions and his results were in very good agreement with the experimental data. Fürth [7] applied the potential (3) to derive the equation of state of a solid phase and found the relationship between the values of the exponents m and n, the value of the energy of sublimation, the isothermal compressibility and the thermal expansion coefficients. Thus m and n may be evaluated from the measurement of the macroscopic parameters of the crystal.

When the interaction of pairs of atoms in L zone co-ordinations is taken into consideration, the energy of a crystal of a pure element may be expressed by the following equation:

$$E^{(L)} = -\frac{N}{2} \sum_{s=1}^{L} z(r_s) V^{(L)}(r_s), \tag{4}$$

where $Z(r_s)$ denotes the co-ordinations number of the s-th zone co-ordinations.

Introducing the potential given by Eq. (3) and substituting for r_s:

$$r_s = a \cdot r_{0s}, \tag{5}$$

where a is the lattice parameter, one obtains:

$$E^{(L)} = -\frac{N}{2}\left[-\frac{A^{(L)}}{a^m} S^{(L,m)} + \frac{B^{(L)}}{a^n} S^{(L,n)} \right], \tag{6}$$

where $S^{(L,m)}$ and $S^{(L,n)}$ denote the lattice sums given by:

$$S^{(L,m)} = \sum_{s=1}^{L} z(r_s) \cdot r_{0s}^{-m},$$

$$S^{(L,n)} = \sum_{s=1}^{L} z(r_s) \cdot r_{0s}^{-n}. \tag{7}$$

The sums depend only on the type of crystalline lattice. The value $E^{(L)}$ calculated with the aid of Eq. (6) is equal to the cohesive energy if the parameter a is substituted by the equilibrium value of the lattice parameter obtained by solving the equation

$$\frac{\partial E^{(L)}}{\partial a} = 0. \tag{8}$$

The solution of Eq. (8) is

$$a_0^{n-m} = \frac{n}{m} \frac{B^{(L)}}{A^{(L)}} \cdot \frac{S^{(L,n)}}{S^{(L,m)}} . \tag{9}$$

Thus the formula for the cohesive energy may be written as follows:

$$\varepsilon = \frac{N}{2} \frac{n-m}{m} \frac{B^{(L)}}{a_0^n} \cdot S^{(L,n)} = \frac{N}{2} \frac{n-m}{n} \frac{A^{(L)}}{a_0^m} \cdot S^{(L,m)}. \tag{10}$$

The above equation may be rewritten as

$$A^{(L)} = A_0^{(L)} \cdot a_0^m \cdot \varepsilon,$$

$$B^{(L)} = B_0^{(L)} \cdot a_0^n \cdot \varepsilon, \tag{11}$$

where

$$A_0^{(L)} = \frac{2n}{N(n-m) \cdot S^{(L,m)}},$$

$$B_0^{(L)} = \frac{2m}{N(n-m) S^{(L,n)}}. \tag{11}$$

It is clear now that it is possible to calculate the parameters of the interaction potential of atoms of a pure component of an alloy with the aid of the measurable values ε and a_0 and Eqs (5), (11).

The next problem is the evaluation of the energy of the interaction of atoms of different elements. Machlin [6] had postulated that the constants of attraction and repulsion A and B of the interaction of different atoms may be estimated directly with the aid of Eqs (11) substituting the cohesive energy ε and the lattice parameter a_0 with the average values $\bar{\varepsilon}$ and $\bar{a}_0$ expressed by the formulae:

$$\bar{\varepsilon} = \frac{\varepsilon_X + \varepsilon_Y}{2},$$

$$\bar{a}_0 = \frac{a_{0X} - a_{0Y}}{2}, \tag{12}$$

where ε_X, ε_Y, a_{0X}, a_{0Y} denote the cohesive energies and lattice parameters of the components X and Y transformed to the uniform structure — "the reference structure" [6] the type of which is determined by the type of the structure of the considered intermetallic phase. Such a transformation may be realized with the aid of Eqs (9), (10). As the lattice sums $S^{(L,m)}$ and $S^{(L,n)}$ depend only on the type on structure, the following relationships may be derived

$$\frac{a_0(\sigma_1)}{a_0(\sigma_2)} = \left[\frac{S_{\sigma_1}^{(L,n)} S_{\sigma_2}^{(L,n)}}{S_{\sigma_1}^{(L,m)} S_{\sigma_2}^{(L,m)}} \right]^{\frac{1}{n-m}}, \tag{13}$$

$$\frac{\varepsilon(\sigma_1)}{\varepsilon(\sigma_2)} = \left[\frac{a_0(\sigma_1)}{a_0(\sigma_2)} \right]^m \frac{S_{\sigma_1}^{(L,m)}}{S_{\sigma_2}^{(L,m)}}, \tag{14}$$

where σ_1 and σ_2 denote the types of structure. Thus knowing the values of the lattice parameter and cohesive energy of an alloy of a given structure, one may calculate the latter parameters of the same substance in another structure — for example in a "reference structure".

Now, we are able to estimate the interaction energies of pairs of atoms of the same and of different elements.

4. The application of the model to the calculation of the phase diagrams of the Heusler alloys $Cu_{3-x}Mn_xAl$ and $Cu_2Mn_{2-y}Al_y$

The energy parameters $W_{ik}(r_s)$ appearing in the formulae (1) and (2) were evaluated by the method described in the previous paragraph. Since the structure of the Heusler alloys in the completely disordered state is of the type A2, the latter type of structure was considered as the "reference structure". In calculating the interaction energies of atoms of single elements the values of the exponents m and n determined by Fürth [5] was applied. For the interaction of the atoms Cu and Al the values $m = 4$, $n = 7$ were used and for the interactions Cu-Mn and Mn-Al the "average" values $m = 4$, $n = 8$ determined by Machlin [6] were used. The lattice parameter was assumed to be constant and independent of the composition of the alloy. The value of the lattice parameter of the alloy Cu_2MnAl was applied and the calculations were done for $a_0 = 5.962$ Å, $L = 2$. Thus the critical

temperature T_1 as a function of the composition of the alloy was determined. Unfortunately the temperatures T_2 were impossible to evaluate since there was no information about the values of the order parameters S_{20} and S_{40}.

The results of our calculations are presented in Tables I and II and Figs 1 and 2.

<div align="right">TABLE I</div>

Values of the lattice parameters a_0, cohesive energies ε^* of crystals of pure elements, calculated values of a_0 and ε in the "reference structure" and calculated values of constants A and B of the interaction potential of similar atoms

Inter-acting atoms	Real structure			Reference structure			A	B
	type	a_0[Å]	$\varepsilon\left[10^{24}\dfrac{eV}{g\,at}\right]$	type	a_0[Å]	$\varepsilon\left[10^{24}\dfrac{eV}{g\,at}\right]$		
Cu	A1	3.607	-2.119	A2	2.911	-1.871	51.487	526.099
Al	A1	4.041	-2.025	A2	3.261	-1.788	77.507	1113.556
Mn	A2	3.081	-1.743	A2	3.081	-1.743	13.205	4817.421

* L. Brever, *Electronic Structure and Alloy Chemistry of the Transition Elements*, ed. by P. Beck, Interscience 1963.

<div align="right">TABLE II</div>

Calculated values of $\bar{a}_0$, $\bar{\varepsilon}$ and of the constants A and B of the interaction potential of atoms of different elements

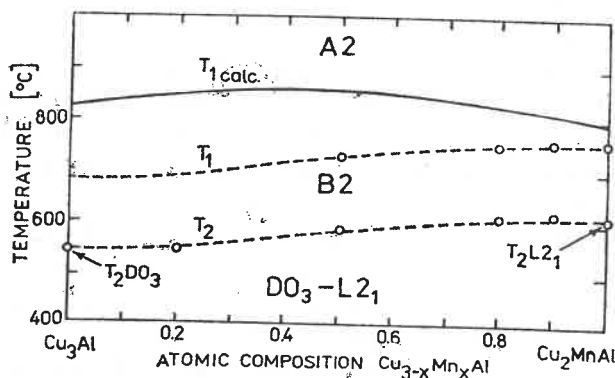| Interacting atoms	Reference structure			A	B
	type	$\bar{a}_0$[Å]	$\bar{\varepsilon}\left[10^{24}\dfrac{eV}{g\,at}\right]$		
Cu-Al	A2	3.086	-1.830	63.596	774.288
Cu-Mn	A2	2.996	-1.807	47.824	1245.524
Mn-Al	A2	3.171	-1.766	58.644	1916.909

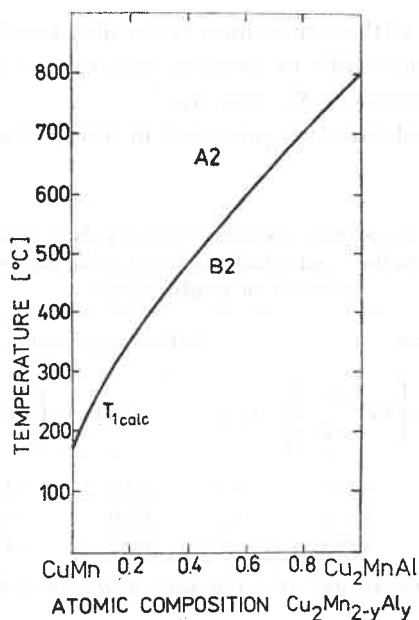Fig. 1. The phase diagram of the alloys $Cu_{3-x}Mn_xAl$. Dashed lines represent the experimental data of Bouchard and Thomas

Fig. 2. The phase diagram of the alloys $Cu_2Mn_{2-y}Al_y$

5. Discussion

In our calculations the simplest formula for the interaction energies of atoms in a crystal was applied. It should be noticed, that among the various known formulae of interaction potentials that one, which was applied in this paper is the only one, which allows us to obtain the simple analytical formulae of the dependence of the configurational energy of an alloy on the number of zone co-ordinations taken into consideration. The main point of our paper is to present a very simple model of the ordering processes of atoms in the cubic, ternary alloys. This was the reason why the Bragg–Williams approximation was applied. It should be also emphasized that this type of interaction potentials was used by Machlin [6] with a great success.

In Fig. 1 the calculated phase diagram of the alloys $Cu_{3-x}Mn_xAl$ is compared with the DTA data of Bouchard and Thomas [8]. The difference between the theoretical and experimental data is less than 15%. In Fig. 2 the phase diagram of the alloys $Cu_2Mn_{2-y}Al_y$ is presented. Unfortunately, hitherto no experimental data on the alloys of such composition have been published.

It should be noted that the lattice parameter of the Heusler alloys $Cu_{3-x}Mn_xAl$ is expected to decrease while x decrease (for Cu_3Al $a_0 = 5.83$ Å, for Cu_2MnAl $a_0 = 5.962$ Å). All the calculations were performed without taking this variation into considerations. The reason was that there was no available information on it.

However, considering the variation of the lattice constant of some binary alloys with varying composition [10, 11] one can expect that if such a variation of the lattice constanst was taken into account in the Heusler alloys $Cu_{3-x}Mn_xAl$ and $Cu_2Mn_{2-y}Al_y$

the difference between the calculated and experimentally obtained dependences of the critical temperature $T_1(x)$ of the alloy would be reduced.

It is interesting to note that the calculated value of the temperature T_1^* is negative for all values of x and y. This indicates that the transition $L2_1 \leftrightarrow A2$ is impossible in the alloys $Cu_{3-x}Mn_xAl$ and $Cu_2Mn_{2-y}Al_y$. In fact, up to now, there is no information about such transitions in the Heusler alloys.

The experimental investigations of the ordering processes of atoms in the Heusler alloys are in progress and the results will be published soon.

We are grateful to Mr. Janusz Wolny for all the numerical calculations and very fruitful discussions.

APPENDIX

The analysis of the applied approximation

The configurational energy of the completely disordered alloys $Cu_{3-x}Mn_xAl$ and $Cu_2Mn_{2-y}Al_y$ was studied as a function of the number of zone co-ordinations in which the interaction of atoms was taken into consideration. The general formula for the configurational energy of a ternary alloy calculated in the approximation of the interaction of atoms in L zone co-ordinations may be written as [9]:

$$E^{(L)} = -\tfrac{1}{2} \sum_{s=1}^{L} \sum_{ik/1}^{3} \sum_{\mu\nu} z_{\mu\nu}(r_s) a_{i\mu} p_{k\nu} V_{ik}(r_s), \tag{15}$$

where $Z_{\mu\nu}(r_s)$ denotes the number of the lattice sites of the kind "ν" surrounding the μ-th lattice site at the distance r_s, $a_{i\mu}$ denotes the number of atoms of the element "i" occupying the μ-th sublattice, $p_{k\nu}$ denotes the probability that an atom of the element "k" occupies any lattice site of the kind "ν". Substituting the potentials $V_{ik}(r_s)$ given by Eq. (3) one obtains:

$$E^{(L)} = -\tfrac{1}{2} \sum_{ik/1}^{3} \left[-A_{ik}^{(L)} \left(\frac{a_0}{2} \right)^{-m} \sum_{\mu\nu} a_{i\mu} p_{k\nu} S_{\mu\nu}^{(L,m)} \right]$$

$$-\tfrac{1}{2} \sum_{ik/1}^{3} \left[B_{ik}^{(L)} \left(\frac{a_0}{2} \right)^{-n} \sum_{\mu\nu} a_{i\mu} p_{k\nu} S_{\mu\nu}^{(L,n)} \right], \tag{16}$$

where:

$$A_{ik}^{(L)} = A_{ik0}^{(L)} [a_0^{(ik)}]^m \cdot \varepsilon_{ik},$$

$$B_{ik}^{(L)} = B_{ik0}^{(L)} [a_0^{(ik)}]^n \cdot \varepsilon_{ik},$$

$$A_{ik0}^{(L)} = \frac{2n}{N(n-m) \cdot S^{(L,m)}},$$

$$B_{ik0}^{(L)} = \frac{2m}{N(n-m) \cdot S^{(L,n)}},$$

$$S_{\mu\nu}^{(L,m)} = \sum_{s=1}^{L} z_{\mu\nu}(r_s) \cdot r_{0s}^{-m},$$

$$S_{\mu\nu}^{(L,n)} = \sum_{s=1}^{L} z_{\mu\nu}(r_s) r_{0s}^{-n},$$

$a_0^{(ik)}$ denotes the "average" lattice parameter given by Eq. (12) applied to the components "i" and "k", a_0 denotes the lattice parameter of the ternary alloy. One should remember that the values of the exponents m and n also depend an the kinds of the interacting atoms. If the expressions for the values $a_{i\mu}$ and $p_{k\nu}$ [2] are substituted into Eqs (15), one will obtain the dependence of the configurational energy $E^{(L)}$ of the long-range order parameters and the composition of the alloy.

The quantitative analysis of the applied approximation was realized for the cases of the alloys discussed in the previous paragraphs. The parameters of composition x and y varied from 0 to 1 with a step of 0.1. To simplify the calculations complete disorder for the atoms was assumed. The results are presented in Figs 3–8. The curves of the pair potential of pure elements calculated for several different values of L are shown in the Figs 3a–c. The values of the configurational energy in three particular cases of the composition of the alloys are presented in Figs 4a–c as functions of L. It is seen that for $L > 10$ the variation of $E^{(L)}$ is practically negligible and that the value of the configurational energy calculated with the consideration of the interaction of atoms in two zones co-ordinations is a very good approximation. Namely, the difference between the value of configurational
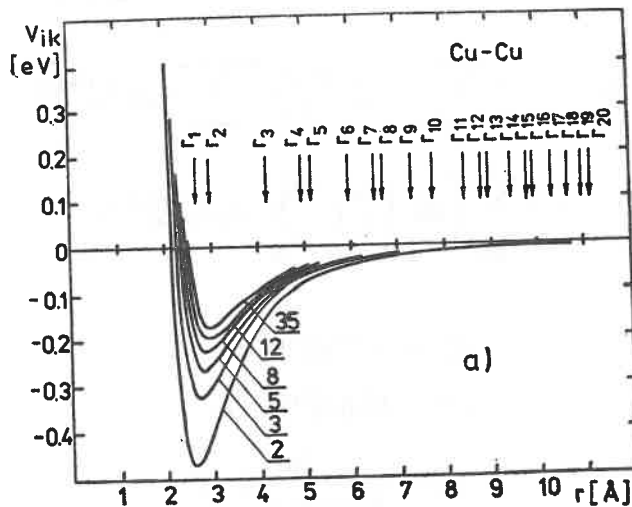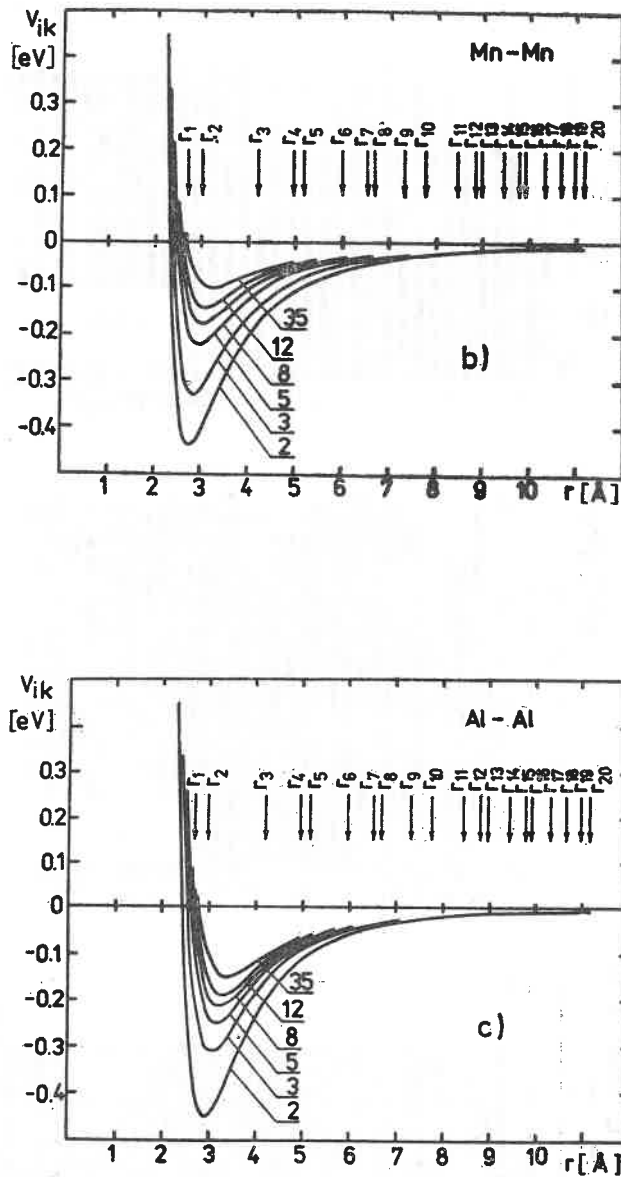
Fig. 3. The interaction potential of atoms of pure elements: a) Cu, b) Mn, c) Al. The curves are specified by the numbers of zone co-ordinations taken into considerations in the calculations of the interaction energy. The radii of the zones co-ordinations in the structure of the Heusler alloys are marked on the "r" axis

energy calculated for two considered zone co-ordinations and the average one obtained with the consideration of more than 10 zone co-ordinations never exceeds 10% (for CuMn about 5%, for Cu_2MnAl about 7.5%, for Cu_3Al 8.5%).
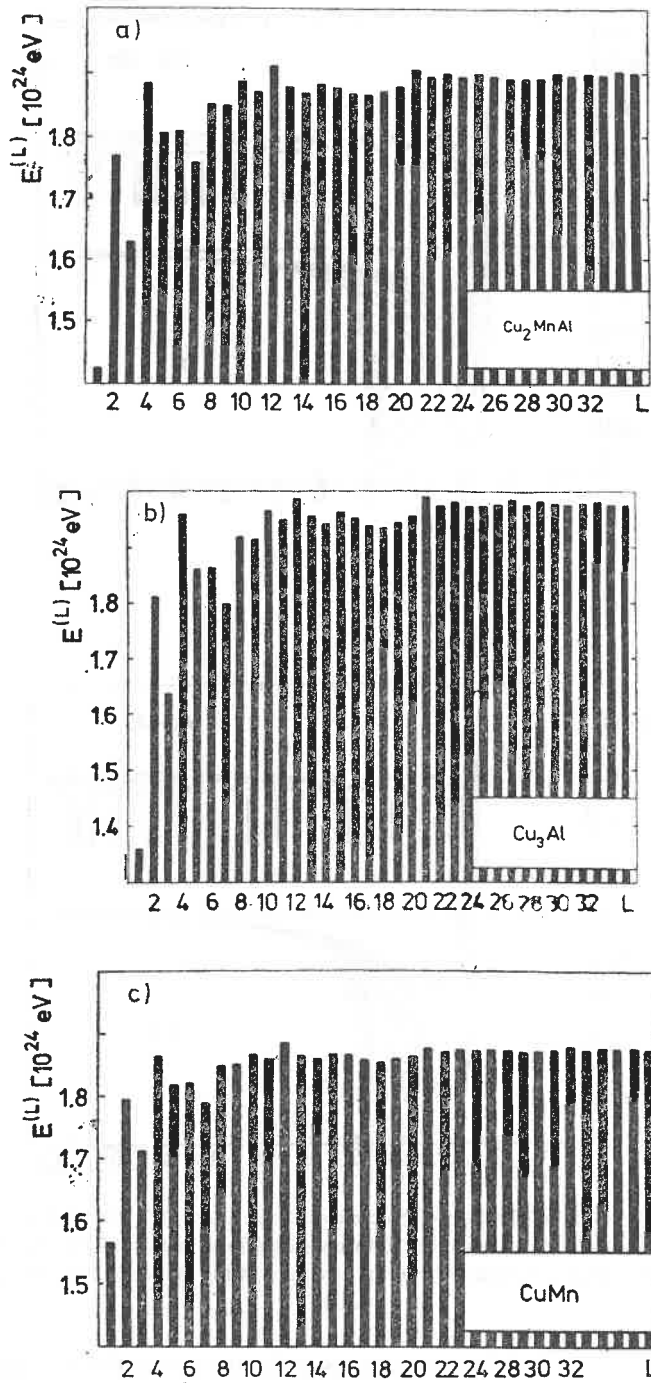
Fig. 4. The configurational energy of the alloys Cu_2MnAl (a), Cu_3Al (b), CuMn (c) as a function of the number of zones co-ordinations taken into consideration in the calculations

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