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THE SITE PREFERENCE ANALYSIS AND ORDERING CHARACTERISTICS OF TERNARY $Cu_{0.5}(Zn_{1-x}M_x)_{0.5}$ (M = TRANSITION METALS) ALLOYS

The site preference of some transition metals during B2-type ordering has been investigated in the ternary $Cu_{0.5}(Zn_{1-x}M_x)_{0.5}$ alloys with M = Ti, V, Ag, Au, Cr, Mn, Fe, Co, Ni, Nb, Mo, Hf, Ta, W, Re or Pt ($x \leq 0.01$). The statistic-o-thermodynamical theory combined with the electronic theory of alloys has been used to calculate the partial ordering energies, partial short range order parameters and the order-disorder transformation temperatures. The values of partial short range order parameters have been used to determine the site preference of the metal M. The analysis shows that the metals M can be divided into two groups with regard to lattice site occupancy. One group comprising of Cr, Mn, Fe, Co, Ni, Nb, Mo, Hf, Ta, W, Re or Pt was found to prefer Zn sublattice sites, while the second group of Ti, V, Ag or Au atoms prefer Cu sublattice sites. It is found that order-disorder transformation temperature and the site preference of metal M both depend strongly on the partial ordering energies and ternary alloying addition of metal M.

Keywords: ternary alloy systems, order-disorder transformations, site occupancy, ab-initio calculations, ordering energies

1. Introduction

Cu-Zn alloys have large industrial, automotive, aerospace and household applications because of their outstanding electrical and thermal conductivities, high corrosion resistance, ease of fabrication, high strength and fatigue resistance [1]. The ordered phase of Cu-Zn alloy is stable at room temperature over a composition range of about 46 to 50 at.% Zn. At high temperatures, its structure is body centred cubic (bcc) with Cu and Zn atoms distributed randomly. Ordering occurs at a temperature of about 733 K (T_c), below which, the corners of the bcc unit cell are occupied by Cu atoms and the center by Zn atom. The ordered alloy therefore has a B2 (CsCl type) structure [2]. Quest for new functional materials with enhanced physical properties, in recent years has lead to research on alloys with ordered structures which exhibit unique properties [3-21].

The effect of ternary addition of transition metals has been recently studied for Cu-Pd & Cu-Pt systems [22]. It has been observed that binary Cu-Pt alloys exhibit $L1_2$-type crystal structures but on ternary addition of transition metals, its structure is changed into cubic ABC_6 type. Cu_3Pd alloy shows disordered face centered cubic crystal structure but on addition of third element i.e. Fe, its structure becomes ordered $L1_2$-type. Physical properties such as electrical, thermal, magnetic and mechanical are influenced by the ternary addition of transition metals [23,36].

But the factors leading to such behavior are still not adequately known. However Ziya et al. [24] have shown that the prediction of such effects can be made with electronic theory of alloys etc.

This paper presents the effect of addition of transition metals on the ordering characteristics of binary Cu-Zn alloys using ab-initio calculations. Partial ordering energies for different pairs of atoms and the normalized transition temperature change has been calculated using statistic-o-thermodynamical theory of atomic ordering combined with the electronic theory of alloys and the data obtained has been used to determine the site preference of the added transition metal in the alloy.

2. Theory

The statistical theory of ordering is based on the quasi-chemical approximation and holds for substitutional ternary ABC-alloys with two types of sites [25]. The procedure involves the calculations of configurational free energy by considering the nearest neighbour interactions and correlation effects. The free energy is minimized with respect to number of different types of atoms on the two types of lattices to obtain the equilibrium values of A, B & C atoms at the first and second lattice sites and the number of pairs of neighbouring atoms. The correlation between any two atoms X and Y in the disordered state in equi-

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librium is defined in terms of a correlation parameter for (AB, AC, BC) atomic pair:

$$\varepsilon_{X'Y'} = \left[\frac{2N_{X'Y'}}{NZ}\right] - c_{X'}c_{Y'} \qquad (1)$$

where N_{XY} is the number of XY-pairs of neighboring atoms and is related to the partial ordering energy W_{XY}. Z is the coordination number. c_X and c_Y are the concentrations of the X and Y atoms, respectively.

The partial short range order (SRO) parameters $\alpha_{XY}(R_i)$ are related to the correlation parameter by [26]:

$$\varepsilon_{X'Y'}(R_i) = -c_{X'}c_{Y'}\alpha_{X'Y'}(R_i) \qquad (2)$$

where R_i is a radius of the ith coordination sphere and for the degree of SRO parameter "α_{XY}".

$\alpha_{XY} = 0$ for randomness,

$\alpha_{XY} < 0$ for SRO,

$\alpha_{XY} > 0$ for clustering.

The calculation of correlation parameter requires ordering energies W_{XY}. The electronic theory of alloys yields the following relation for the partial ordering energies W_{XY} [25]:

$$W_{X'Y'}(R_i) = \frac{\overline{\Omega}_0}{\pi^2}\int_0^\infty F_{X'Y'}(q)\frac{\sin qR_i}{qR_i}q^2 dq \qquad (3)$$

$$F_{X'Y'}(q) = -\frac{\overline{\Omega}_0}{8\pi}\left|\omega_{X'}^0(q) - \omega_{Y'}^0(q)\right|^2 q^2 \frac{\varepsilon(q)-1}{\varepsilon^*(q)} + $$
$$+ \frac{2\pi}{\overline{\Omega}_0 q^2}\left|Z_{X'}^* - Z_{Y'}^*\right|^2 \exp\left(-\frac{q^2}{4\eta}\right) \qquad (4)$$

where $\overline{\Omega}_0$ is the average atomic volume of the ternary alloy; $\varepsilon(q)$ is the dielectric function in the Hartree approximation, $\varepsilon^*(q)$ is the modified dielectric function which takes into account the correlation and exchange effects, $\omega_{X'}^0(q)$ and $\omega_{Y'}^0(q)$ are the form factors of unscreened pseudopotentials of X' and Y' ions, $Z_{X'}^*$ and $Z_{Y'}^*$ are the effective valencies of the X' and Y' atoms respectively. η is the Ewald's parameter [27]. Its value was taken as $\eta = 0.1$.

The relation between the order-disorder (O-D) transformation temperature, T_o, and the long range order (LRO) parameter, S, for B2-type ordered binary alloys can be obtained by the application of method of static concentration waves [28]:

$$\ln\left[\frac{\left(c_B + \frac{1}{2}S\right)\left(c_A + \frac{1}{2}S\right)}{\left(c_B - \frac{1}{2}S\right)\left(c_A - \frac{1}{2}S\right)}\right] = \frac{1}{k_B T}SW(\vec{K}_o) \qquad (5)$$

and

$$T_o = -\frac{c_A c_B}{k_B}W(\vec{K}_o) \qquad (6)$$

where $W(K_o)$ is the ordering energy for $\vec{K}_o = 2\pi\left(\vec{a}_1^* + \vec{a}_2^* + \vec{a}_3^*\right)$, the shortest wave vector and $\vec{a}_n^*$ are the reciprocal lattice vectors. $W(Ko)$ in the case of B2-type superstructure is related to $W(R_i)$ by [25]:

$$\begin{aligned}W(R_i) &= 8W(R_1) - 6W(R_2) - 12W(R_3) + \\ &+ 24W(R_4) - 8W(R_5) + \ldots\ldots\ldots\end{aligned} \qquad (7)$$

The calculation of temperature "T_o" requires the values of ordering energies corresponding to the first five coordination spheres. The change in O-D phase transformation temperature, $\Delta T = T_{oc} - T_o$, upon addition of a small concentration of the metal M to the binary B2-type ordered alloy, is given by [29]:

$$\Delta T \approx 49c_C\left[1 - \frac{49}{48\cosh^2\left(\frac{W_{AC} - W_{BC}}{4k_B T_o}\right)}\right]T_0 \qquad (8)$$

The effect of ternary addition of metal M can be readily seen from the transformation temperature change ΔT^1 as it depends on the partial ordering energies $W(R_i)$.

3. Results and discussion

The validity of the theory on binary CuZn alloys has to be checked prior its application to the ternary $Cu_{0.5}(Zn_{1-x}M_x)_{0.5}$ alloys. Fig. 1 shows the plot of ordering energy against the radial distance for the binary CuZn alloy. The dependence of the ordering energy on the radial distance is semi-oscillatory and has a sign changing character, observed usually for alloys. Such a dependence of ordering energy on radial distance can be attributed to electron concentration (e/a) and the composition of the alloy [30]. The calculated values of ordering energies are given in Table 1 along with the experimental values of T_o. The calculated value of the O-D phase transformation temperature of binary CuZn alloy is in a good agreement with the experimental value.
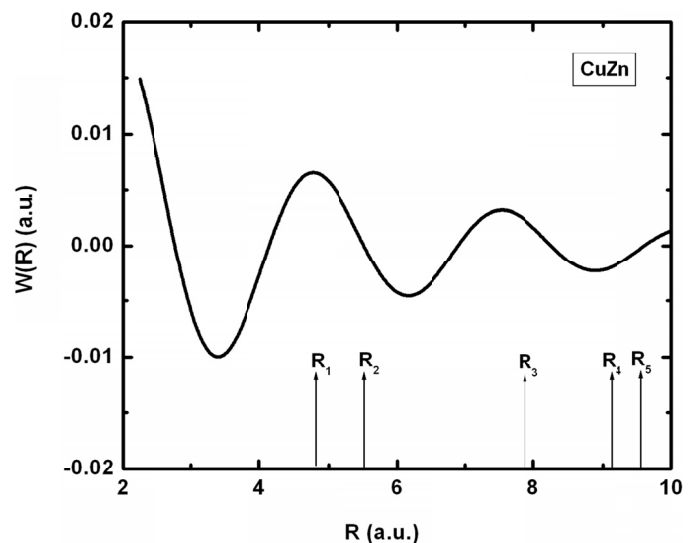

Fig. 1. The dependence of ordering energy on radial distance for CuZn alloy (1 a.u. of energy = 27.2 eV and 1 a.u. of length = 0.529Å)

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[1] Where $\Delta T = (T_{oc} - T_o)$ and T_{oc} is the O-D transformation temperature of ternary alloys.

TABLE 1

The calculated ordering energies $W(R_i)$ for the first five coordination spheres and the O-D transformation temperatures T_o, in Kelvin (K) for the binary CuZn alloy

Alloy	$W(R_1)$ (a.u.)	$W(R_2)$ (a.u.)	$W(R_3)$ (a.u.)	$W(R_4)$ (a.u.)	$W(R_5)$ (a.u.)	T_o(Cal.) (K)	T_o(Exptl.) (K) [31]
CuZn	6.49×10^{-3}	-7.32×10^{-4}	2.20×10^{-3}	-1.54×10^{-3}	2.56×10^{-4}	713 ± 10	741

Fig. 2 shows the dependence of partial ordering energies $W_{Cu-M}(R_1)$ and $W_{Zn-M}(R_1)$ on the radial distance for $Cu_{0.5}(Zn_{1-x}M_x)_{0.5}$ ternary alloys with M = Ti and W. The radius of the first coordination sphere is indicated by an arrow in the figure. The coordination radii for the $Cu_{0.5}(Zn_{1-x}M_x)_{0.5}$ alloys do not differ much from those for the binary CuZn alloy because the concentration of the metal M was very small. The dependence of the ordering energy on radial distance has a semi-oscillatory and sign changing nature similar to the binary CuZn alloy. The ordering energies for the different pairs of atoms differ in magnitude. The values of partial SRO parameters corresponding to a temperature of 673 K were determined using Eq. (2).
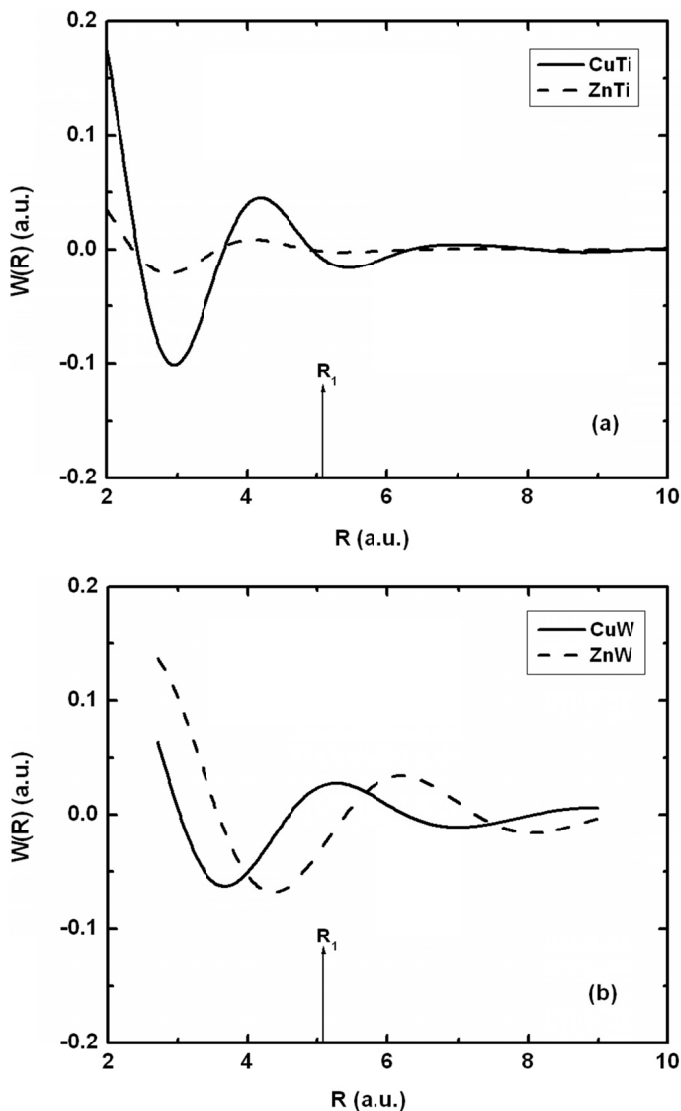

Fig. 2. The dependence of ordering energy on radial distance for $Cu_{0.5}(Zn_{1-x}M_x)_{0.5}$ ternary alloys. The ordering energies are shown for (a) Cu-Ti and Zn-Ti (b) Cu-W and Zn-W atomic pairs

The values of the partial SRO parameters calculated using the aforementioned method are given in Table 3 for Cu-Zn, Zn-M and Cu-M pairs. The experimental data on partial SRO parameters for these pairs is scarcely available, however available experimental data agree well with the calculated data with regard to their sign as shown in Table 3.

The partial SRO parameters for the Cu-M pairs with M = Cr, Mn, Fe, Co, Ni, Nb, Mo, Hf, Ta, W, Re or Pt, have a negative sign ($\alpha_{Cu-M}(R_1) < 0$) and Zn-M pairs have a positive sign ($\alpha_{Zn-M}(R_1)$) (see Table 2 and 3). Further, the magnitude of the SRO parameters $\alpha_{Zn-M}(R_1)$ for M = Cr, Mo, W, Re or Pt are nearly 20 times, for M = Nb or Ta are nearly 15 times and for M = Mn or Hf are nearly 10 times higher than those of M = Fe, Co and Ni in these alloys. It is thus assumed that the atoms of M = Cr, Mn, Nb, Mo, Hf, Ta, W, Re or Pt substitute exclusively for Zn sublattice sites and are surrounded by Cu atoms. However, in the case of M = Fe, Co and Ni, the $\alpha_{XY}(R_1)$ parameter has the same sign (negative) for Cu-M pairs and positive sign for Zn-M pairs as for M = Cr, Mn, Nb, Mo, Hf, Ta, W, Re or Pt atoms, but they differ in magnitudes. This shows that M = Fe, Co or Ni atoms substitute preferentially for the Zn sublattice sites and are surrounded by Cu atoms.

TABLE 2

Partial ordering energies of $Cu_{0.5}(Zn_{1-x}M_x)_{0.5}$ alloys, for x = 0.01 at the first coordination sphere. Ordering energy for CuZn pair, $W_{CuZn}(R_1) = 2.482 \times 10^{-3}$ a.u

Elements	Ordering energies (a.u.)	
	W_{Zn-M}	W_{Cu-M}
Ti	-2.024×10^{-3}	-1.074×10^{-2}
V	8.753×10^{-4}	-1.864×10^{-2}
Ag	5.131×10^{-3}	-3.950×10^{-4}
Au	4.004×10^{-3}	-3.577×10^{-3}
Cr	-5.950×10^{-2}	3.423×10^{-3}
Mn	-7.232×10^{-3}	6.483×10^{-4}
Fe	2.766×10^{-3}	3.481×10^{-3}
Co	-5.920×10^{-5}	6.656×10^{-4}
Ni	2.060×10^{-6}	6.867×10^{-4}
Nb	-1.039×10^{-2}	4.329×10^{-3}
Mo	-1.097×10^{-2}	3.017×10^{-2}
Hf	-4.789×10^{-3}	4.421×10^{-3}
Ta	-7.644×10^{-3}	4.673×10^{-3}
W	-2.194×10^{-2}	2.670×10^{-2}
Re	2.845×10^{-2}	4.933×10^{-2}
Pt	-1.079×10^{-2}	1.035×10^{-2}

TABLE 3

Partial SRO parameters $\alpha_{X'Y'}(R_1)$ for $Cu_{0.5}(Zn_{1-x}M_x)_{0.5}$ alloys, for x = 0.01 at T = 673 K

Ele-ments	Partial SRO parameters					
	α_{CuZn}	Exptl. [32]	α_{Zn-M}	Exptl.	α_{Cu-M}	Exptl.
Ti	–0.181	–0.171 to –0.182	–0.547	—	0.569	—
V	–0.181	-"-	–0.887	—	0.892	—
Ag	–0.181	-"-	–0.392	—	0.381	(+) [33]
Au	–0.181	-"-	–0.512	—	0.503	—
Cr	–0.181	-"-	0.999	—	–0.987	—
Mn	–0.181	-"-	0.523	—	–0.511	(–) [34]
Fe	–0.181	-"-	0.049	(+) [37]	–0.055	—
Co	–0.181	-"-	0.052	—	–0.053	—
Ni	–0.181	-"-	0.048	—	–0.050	—
Nb	–0.181	-"-	0.793	—	–0.787	—
Mo	–0.181	-"-	0.995	—	–0.995	—
Hf	–0.181	-"-	0.588	—	–0.586	—
Ta	–0.181	-"-	0.718	—	–0.714	—
W	–0.181	-"-	0.998	—	–0.998	—
Re	–0.181	-"-	0.910	—	–0.911	—
Pt	–0.181	-"-	0.914	—	–0.913	(-) [35]

For M = Ti, V, Ag or Au, the $\alpha_{XY}(R_1)$ parameters have a positive sign for the Cu-M pairs and a negative sign for Zn-M atomic pairs. Therefore, the atoms of these metals substitute mainly for the Cu sublattice sites and are surrounded by Zn atoms in the CuZn alloy. A comparison of the magnitudes of $\alpha_{XY}(R_1)$ shows that the probability of substitution for Cu-sublattice sites by V atoms is higher than that of Ti, Ag and Au atoms. Thus it is concluded that the arrangement of atoms of the metal M over Cu and Zn sublattices in $Cu_{0.5}(Zn_{1-x}M_x)_{0.5}$ alloy is determined by the magnitude and sign of the partial ordering energy. It is important to note that, the sign of the short range order parameter involves the distribution of third alloying atoms over the sublattices of Cu and Zn in Cu-Zn alloys and the magnitude of short range order parameter provides valuable information on the bond strengths of atomic pairs of Cu-X or Zn-X relative to Cu-Zn in $Cu_{0.5}(Zn_{1-x}M_x)_{0.5}$ alloys [38]. The value of lies within the range obtained from experiments (see Table 3).

The estimated change in the O-D transformation temperature ΔT that occurs on addition of the metal M in $Cu_{0.5}(Zn_{1-x}M_x)_{0.5}$ alloy is given in Table 4 for x = 0.25 at.%, 0.5 at.% and 1 at.%. It is observed that the O-D transformation temperature either increases or decrease on the addition of metal M to the binary CuZn alloy. The increase or decrease in the O-D transformation temperature is due to their dependence on the ordering energies and on the ternary alloying elements M [38].

It is obvious from Table 4 that the metal M in $Cu_{0.5}(Zn_{1-x}M_x)_{0.5}$ can be divided into two groups on the basis of the absolute values of partial ordering energies $W_{Cu-M}(R_1)$ and $W_{Zn-M}(R_1)$:

i) For M = V, Cr, Nb, Mo, W, Re or Pt, the absolute values of partial ordering energies $W_{Cu-M}(R_1)$ and $W_{Zn-M}(R_1)$ are

close to or greater than the $W_{CuZn}(R_1)$. These additions lead to a large increase in the value of T_{oc}. This increase in T_{oc} is seen to increase rapidly with the increase in the concentration of the metal M, except Ti, for which increase in T_{oc} is not so large, yet it is rapid with the increase in concentration.

ii) For M = Ag, Fe, Co, Ni, Hf and Ta, the absolute values of the partial ordering energies $W_{Cu-M}(R_1)$ and $W_{Zn-M}(R_1)$ are though close to or less than $W_{CuZn}(R_1)$, but their addition leads to less increase in the value of T_{oc} as compared to the first group of metals. Further, the increase in T_{oc} has the same ratio as the ratio of the metal M.

TABLE 4

The percentage temperature change ($\Delta T\%$) calculated for $Cu_{0.5}(Zn_{1-x}M_x)_{0.5}$ alloys, at various impurity levels x (in at. %). (T_o = 741 K for CuZn alloy [31])

Elements	Temperature change ΔT (%)		
	x = 0.25%	x = 0.5%	x = 1%
Ti	3.198	6.395	12.787
V	5.742	11.485	22.973
Ag	1.756	3.419	6.467
Au	2.793	5.429	10.633
Cr	6.124	12.249	24.499
Mn	2.803	5.608	11.217
Fe	–0.092	–0.184	–0.366
Co	–0.091	–0.181	–0.362
Ni	–0.094	–0.189	–0.378
Nb	5.125	10.247	20.487
Mo	6.121	12.242	24.448
Hf	3.446	6.865	13.664
Ta	4.546	9.090	18.170
W	6.124	12.248	24.496
Re	5.836	11.673	23.348
Pt	5.850	11.702	23.409

It is inferred from the present study that the O-D transformation temperature either increases or remains unchanged on the ternary addition of various transition metals to the binary CuZn alloy depending upon the absolute values of partial ordering energies of different pairs of atoms. The type and nature of the ternary additions has a significant effect on the O-D transformation temperature. Further, the ternary elements corresponding to which magnitude of partial SRO parameter is large, a significant increase in the O-D transformation temperature is observed.

4. Conclusions

It can be concluded from the present study that:

1. The metal M in $Cu_{0.5}(Zn_{1-x}M_x)_{0.5}$ alloys can be divided into two main groups on the basis of the lattice site occupancy: The ($\alpha_{Zn-M}(R_1) > 0$) for the Zn-M pair with M = Cr, Mn, Fe, Co, Ni, Nb, Mo, Hf, Ta, W, Re or Pt, which shows that

these elements mainly substitute Zn sublattice sites and are surrounded by Cu atoms.

The $(\alpha_{\text{Cu-M}}(R_1) > 0)$ for M = Ti, V, Ag or Au which shows that these metals mainly substitute Cu sublattice sites and are surrounded by Zn atoms.

2. The ternary addition to CuZn alloy leads to either an increase or decrease in O-D transformation temperature depending upon the absolute value of partial ordering energies of different atomic pairs and ternary alloying addition.

For M = Ti, V, Cr, Nb, Mo, W, Re or Pt, the absolute value of partial ordering energies $W_{\text{Cu-M}}(R_1)$ and $W_{\text{Zn-M}}(R_1)$ are close to or greater than $W_{\text{CuZn}}(R_1)$, the increase in T_{oc} is large and rapid and has nearly the same ratio as the ratio of metal M.

For M = Ag, Au, Mn, Fe, Co, Ni, Hf or Ta, the absolute values of partial ordering energies of $W_{\text{Cu-M}}(R_1)$ and $W_{\text{Zn-M}}(R_1)$ are close to or less than $W_{\text{CuZn}}(R_1)$, the increase in T_{oc} is slow and has nearly the same ratio as the ratio of metal M.

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