PATTERN RECOGNITION APPLIED TO HEAT OF MIXING OF LIQUID ALLOYS①

Li, Chonghe Li, Ming Tang, Bo Huang, Shiping Zhang, Weiming Chen, Nianyi
Shanghai Institute of Metallurgy, Academia Sinica, Shanghai 200050, China

ABSTRACT

By pattern recognition, artificial neural network and chemical bond parameter method, the regularities of liquid alloys have been found, with their physical meaning discussed.

Key words: liquid alloys heat of mixing pattern recognition

In our previous works, the relationships of chemical bond parameters and the entropy of liquid alloys have been investigated[1]. In this work, pattern recognition, artificial neural network and chemical bond parameters are used together to investigate the regularities of the heat of mixing of liquid alloys.

Fig. 1 illustrates the result of the classification of liquid binary alloys consisting of two nontransition metals according to the sign of their heat of mixing[2] (the exothermic mixing or endothermic mixing). The parameters used are $\triangle(Z/R^3)$, $\triangle X$, $\Sigma(n+r)$. Here Z is the number of valance electrons of atoms. R is the metallic radius. $\triangle(Z/R^3)$ is the difference of (Z/R^3) of both component atoms, $\triangle X$ is the difference of electronegativities of both component atoms. n and r are the row number and column number of elements in periodic table respectively. The sum of $(n+r)$ of both component atoms is $\Sigma(n+r)$. From Fig. 1 it can be seen that the alloys with positive $\triangle H_{mixing}$ and that with negative $\triangle H_{mixing}$ distribute in different regions, with clear boundary between them.

Artificial neural networks can also be used to investigate the regularities of the heat of mixing of liquid alloys. A three layered artificial neural network with three hidden nodes is used for classification. The inputs used are $\triangle(Z/R^3)$, $\triangle X$, $\Sigma(n+r)$ tan hx is used as the transfer function. The program of Neural Ware Inc. is used. After training the artificial network can be used to classify correctly alloys according to the sign of $\triangle H_{mixing}$.

For the transition metal-containing binary alloys, the regularity of the heat of mixing is different from that of non-transition metal alloys. But for systems containing one definite transition metal the alloys systems with positive $\triangle H_{mixing}$ and negative $\triangle H_{mixing}$ can also be classified by using Z/R^3, X, and Z of another metal element. Here Z is the valance electron number, R is the metallic radius and X is the electronegetivity of elements. Fig. 2 is the Ag-containing binary alloys systems classified according to the heat of mixing. The alloy systems with positive H_{mixing} and those with negative

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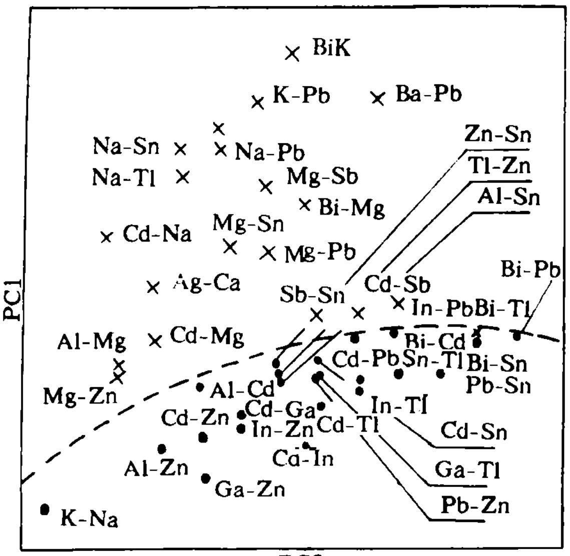

Fig. 1 The relationship of chemical bond parameters and the heat of mixing of nontransition metal liquid alloys (PCA Method). (The data has been normalized)

•—The heat of mixing is negative;

×—The heat of mixing is positive and greater than 2090 J/mol

$PC1 = 0.45\triangle(Z/R^3) + 0.89\triangle X - 0.96\Sigma(n+r)$

$PC2 = 0.89\triangle(Z/R^3) - 0.84\triangle X + 0.85\Sigma(n+r)$

H_{mixing} distribute in different regions.

Z/R^3 roughly represents the density of distribution of valance electron of element. X roughly represents charge transfer in alloys. Those two parameters are related to the bonding energy of metals or alloys. the physical meaning of $(n+r)$ is not very clear yet. Perhaps it is related to relative effect since this parameter becomes siginificant for heavy elements.

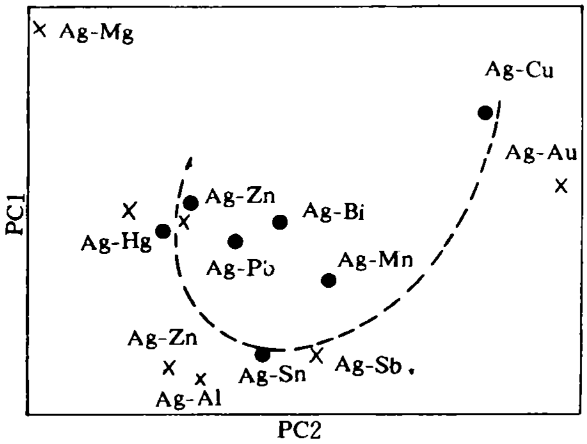

Fig. 2 The distributing regularity of the Ag-containing binary alloys systems classified according to the heat of mixing (PCA method). (The data has been normalized)

•—The heat of mixing is negative;

×—The heat of mixing is positive.

$PC1 = 0.63(Z/R^3) + 0.50X - 0.59Z$

$PC2 = 0.75(Z/R^3) - 0.18X + 0.64Z$

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