ESTABLISHMENT AND APPLICATIONS OF MATHEMATICAL MODELS FOR CONCENTRATION DISTRIBUTIONS IN Mo-Fe-Ni-Co DIFFUSION QUARTERNARY

(Ⅰ) Establishment of Mathematical Models①

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ABSTRACT By means of a Mo-Fe-Ni-Co diffusion quarternary and the B-type spline functions, the mathematical models of the components have been established on the two-dimensional plane of the diffusion quarternary for the six single-phase regions δ-MoNi, *P*, μ-Fe_7Mo_6, *bcc*(Fe), *bcc*(Mo) and *fcc* in the Mo-Fe-Ni ternary system, and for the four single-phase regions δ-MoNi, μ-Co_7Mo_6, *bcc*(Mo) and *fcc* in the Mo-Ni-Co ternary system.

Key words Mo-Fe-Ni-Co diffusion quarternary mathematical models concentration distribution B-type spline functions

1 INTRODUCTION

The diffusion couple technique has found wide applications in the study of phase diagrams at home and abroad. However those applications are limited to measuring a ternary isothermal section with a diffusion triple, measuring a quarternary isothermal tetrahedron with a diffusion quarternary, and studying the concentration distribution in one-dimension. Previously, the authors have measured the isothermal sections at 1 200 ℃ in the Mo-Fe-Ni and Mo-Ni-Co ternary systems with a Mo-Fe-Ni-Co diffusion quarternary simultaneously[1, 2], which is beneficial to make an overall study of the phase equilibrium relations of the two related ternary systems, and to raise the efficiency of phase diagram measurement. This work is aimed at giving a comprehensive description of the atomic diffusions in the Mo-Fe-Ni-Co diffusion quarternary, and establishing mathematical models for the concentration distributions of the components on the two-dimensional plane of the diffusion quarternary, thus helping determine the concentration distribution of each component by means of calculation and display all the phase equilibria in the diffusion quarternary.

2 SETTING-UP OF COORDINATION SYSTEM

The rectangular coordinate systems are set up to describe the phase region distributions at 1 200 ℃ of the Mo-Fe-Ni and Mo-Ni-Co ternary systems in the Mo-Fe-Ni-Co diffusion quarternary[1, 2], as shown in Figs. 1, 2. In the figures, the *z* axis expresses the concentration. Mathematical models of concentration distribu-

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tions can be established using the data in Figs. 1, 2 obtained from EPMA, thus the mole fractions of Mo, Fe, Ni and Co components at any point can be calculated.

3 SELECTION OF MATHEMATICAL METHOD – B-TYPE SPLINE FUNCTION

Fig. 2 Schematic diagram of phase regions in Mo-Ni-Co ternary system

Take the δ-MoNi phase region in Fig. 1 as an example. Assuming the concentration of Fe at point (x, y) is z%, then z depends on x and y, thus z is a function of x and y, i. e. $z = F(x, y)$. The concentration profile of Fe can be established by changing (x, y) in the δ-MoNi phase region, which is a curved surface located above this region. Let the surface be α. Draw a straight line l parallel to x axis containing l perpendicular to xOy plane. Use Γ to express the intersection line of those two planes. Γ is a concentration curve, which can depict the whole curved surface of concentration when line l moves up and down in the δ-MoNi region. Because $z = F(x, y)$ is unknown, P is unknown. If we can know the P curve corresponding to each line l, then we can know the curved surface α, thus obtaining the concentration $z = F(x, y)$ required.

P is curved macroscopically, but the small segments cut from Γ are microscopically straight. Using straight line segments to take the place of corresponding curved segments microscopically and connecting them, a broke line can be obtained. By polishing this broken line macroscopically, a smooth curve can be obtained. Through approximation treatment, this smooth curve can be used to express curve Γ. In this work, the B-type spline functions with good integral approximation and shape preserving property are adopted in the polishing treatment of the broken line[3, 4].

4 ESTABLISHMENT OF MATHEMATICAL MODELS OF CONCENTRATION DISTRIBUTIONS

4.1 Mo-Fe-Ni ternary system

First, establish the mathematical model of concentration distributions of Mo, Ni and Fe in the δ-MoNi region, then the other regions can be treated similarly. Consider the concentration distributions along the straight line segments 40 – 17, 41– 18, 42– 19, 43– 20, 44– 21, 45– 22 in Fig. 1. It is known from Ref. [1] that the concentrations of Mo and Ni almost change linearly along the directions parallel to y axis, therefore linear interpolation equations can be used to calculate the concentration distributions along those segments. Let y_i and z_i stand for the ordinate and concentration of point i, then the concentration z along the above six straight line segments with ordinate y can be expressed as

40– 17:

$$z = z_{17} + \frac{z_{40} - z_{17}}{y_{40} - y_{17}}(y - y_{17}) \tag{1}$$

41– 18:

$$z = z_{18} + \frac{z_{41} - z_{18}}{y_{41} - y_{18}}(y - y_{18}) \tag{2}$$

42– 19:

$$z = z_{19} + \frac{z_{42} - z_{19}}{y_{42} - y_{19}}(y - y_{19}) \tag{3}$$

43– 20:

$$z = z_{20} + \frac{z_{43} - z_{20}}{y_{43} - y_{20}}(y - y_{20}) \tag{4}$$

44– 21:

$$z = z_{21} + \frac{z_{44} - z_{21}}{y_{44} - y_{21}}(y - y_{21}) \tag{5}$$

45– 22:

$$z = z_{22} + \frac{z_{45} - z_{22}}{y_{45} - y_{22}}(y - y_{22}) \tag{6}$$

Because the right boundary of the δ-MoNi region is a curved line segment 46– 23, the concentration along it cannot be calculated using linear interpolation. Now, introduce an assumed point 23′, as shown in Fig. 3. Because point C is on the straight line segment 45– 22, its concentration can be obtained from eq. (6). Suppose the δ-MoNi region extends to straight line segment 46– 23′. Due to the fact that the straight line segment C– 23′ is very short, the concentration variation along C– 23′ can be considered

Fig. 3 Schematic diagram of linear interpolation

as linear. Therefore, using the data at points C and 23, the concentration at point $23'$ can be calculated by means of linear interpolation, i. e. $z_{23'}$: Mo, 47. 10; Ni, 40. 44; Fe, 12. 16. Then the concentration along straight line segment $46-23'$ is

$46-23'$:

$$z = z_{23'} + \frac{z_{46} - z_{23'}}{y_{46} - y_{23'}}(y - y_{23'}) \qquad (7)$$

Draw a straight line l paralled to x axis in the δ-MoNi region(ordinate= y), then the abscissa of the intersection points of l and straight line segments 40– 17, 41– 18, 42– 19, 43– 20, 44– 21, 45– 22, $46-23'$ are respectively – 160, – 140, – 120, – 100, – 80, – 60, – 40. Take y = 20 as an example. Let z_i and $z_{23'}$ in eqs. (1) ~ (7) express the concentration of Fe, then the values at those intersection points are 1. 92, 3. 54, 4. 94, 6. 13, 8. 96, 9. 78, 11. 50. Taking l as abscissa axis, set up $lO'z$ rectangular coordinate system(see Fig. 4)

Fig. 4 Schematic diagram of mathematical polishing for broken line AB

and connect the above 7 points, then a broken line of concentration, AB, is obtained, which can approximately replace the concentration curve Γ. The mathematical expression of AB is

$$z = F_1(x,\ 20) = 1.92M_2\left(\frac{x+160}{20}\right) + 3.54M_2\left(\frac{x+140}{20}\right) + 4.94M_2\left(\frac{x+120}{20}\right) + 6.13M_2\left(\frac{x+100}{20}\right) + 8.96M_2\left(\frac{x+80}{20}\right) + 9.78M_2\left(\frac{x+60}{20}\right) + 11.50M_2\left(\frac{x+40}{20}\right)$$

where $M_2(x)$ is a second - order standard B-type spline function, and

$$M_2(x) = (\delta D^{-1})M_1(x)$$

$$M_1(x) = \delta x_+^0$$

D is a differential operator and δ is a central differential quotient operator with a step of 1, $M_1(x)$ is a first-order standard spline function, and

$$x_+^k = \begin{cases} x^k, & x > 0 \\ 0, & x \leqslant 0 \end{cases}$$

The derivative variation of concentration is continuous, therefore, the concentration curve P is smooth. In order to make the concentration broken line AB approximate P, it is necessary to make mathematical polishing treatment for AB. In order to make the polished curve pass the end points A and B, it is reasonable to extend A to A' and B to B', and $x_A - x_{A'} = x_{B'} - X_B = 20$ μm, then $z_{A'} = 2 \times 1.92 - 3.54 = 0.3$, $z_{B'} = 2 \times 11.50 - 9.78 = 13.22$. Consequently, the mathematical expression of the broken line $A'B'$ is

$$z = F_2(x,\ 20) = 0.3M_2\left(\frac{x+180}{20}\right) + F_1(x,\ 20) + 13.22M_2\left(\frac{x+20}{20}\right)$$

After carrying out a mathematical polishing on $A'B'$, we can obtain the concentration curve Γ corresponding to $l(y = 20)$:

$$\begin{aligned} z = F(x,\ 20) &= \frac{\delta_{20}}{20}D^{-1}F_2(x,\ 20) \\ &= 0.3\frac{\delta_{20}}{20}D^{-1}M_2\left(\frac{x+180}{20}\right) + \frac{\delta_{20}}{20}D^{-1}F_1(x,\ 20) + 13.22\frac{\delta_{20}}{20}D^{-1}M_2\left(\frac{x+20}{20}\right) \\ &= 0.3M_3\left(\frac{x+180}{20}\right) + 1.92M_3\left(\frac{x+160}{20}\right) + 3.54M_3\left(\frac{x+140}{20}\right) + 4.94M_3\left(\frac{x+120}{20}\right) + \\ &\quad 6.13M_3\left(\frac{x+100}{20}\right) + 8.96M_3\left(\frac{x+80}{20}\right) + 9.78M_3\left(\frac{x+60}{20}\right) + 11.50M_3\left(\frac{x+40}{20}\right) + \end{aligned}$$

$$13.22 M_3\left(\frac{x+20}{20}\right)$$
$$= 0.3 M_3\left(9+\frac{x}{20}\right)+ 1.92 M_3\left(8+\frac{x}{20}\right)+3.54 M_3\left(7+\frac{x}{20}\right)+ 4.94 M_3\left(6+\frac{x}{20}\right)+6.13 M_3\left(5+\frac{x}{20}\right)+ 8.96 M_3\left(4+\frac{x}{20}\right)+9.78 M_3\left(3+\frac{x}{20}\right)+ 11.50 M_3\left(2+\frac{x}{20}\right)+13.22 M_3\left(1+\frac{x}{20}\right) \quad (8)$$

where $\frac{\delta_{20}}{20}$ is a central differential quotient operator with a step of 20 μm, $M_3(x)$ is a third-order B-type standard spline function:

$$M_3(x) = (\delta D^{-1})^2 M_1(x)$$

Noting the characteristics of δ and D^{-1}, we get

$$M_3(x) = (\delta D^{-1})^2 \delta x_+^0 = \delta^3 D^{-2} x_+^0 = \frac{1}{2}\delta^3 x_+^2$$

Because

$$\delta^3 = (E^{1/2} - E^{-1/2})^3 = (I - E^{-1})^3 E^{3/2} = \sum_{j=0}^{3}(-1)^j \binom{3}{j} E^{-j+3/2}$$

where E is a displacement operator, I is an identical operator, we get

$$M_3(x) = \frac{1}{2}\sum_{j=0}^{3}(-1)^j\binom{3}{j}E^{-j+3/2}x_+^2 = \frac{1}{2}\sum_{j=0}^{3}(-1)^j\binom{3}{j}\left(x+\frac{3}{2}-j\right)_+^2$$
$$= \begin{cases} 0.75 - x^2 & (|x| < 0.5) \\ 0.5x^2 - 1.5|x| + 1.125 & (0.5 \leqslant |x| < 1.5) \\ 0 & (|x| \geqslant 1.5) \end{cases} \quad (9)$$

Similar to the treatment of eq. (8), we obtain the concentration curve corresponding to l in the δ-MoNi region:

$$z = S(x, y) = \left[2z_{17} + 2\frac{z_{40}-z_{17}}{y_{40}-y_{17}}(y-y_{17}) - z_{18} - \frac{z_{41}-z_{18}}{y_{41}-y_{18}}(y-y_{18})\right]M_3\left(9+\frac{x}{20}\right)+$$
$$\left[z_{17}+\frac{z_{40}-z_{17}}{y_{40}-y_{17}}(y-y_{17})\right]M_3\left(8+\frac{x}{20}\right)+$$
$$\left[z_{18}+\frac{z_{41}-z_{18}}{y_{41}-y_{18}}(y-y_{18})\right]M_3\left(7+\frac{x}{20}\right)+$$
$$\left[z_{19}+\frac{z_{42}-z_{19}}{y_{42}-y_{19}}(y-y_{19})\right]M_3\left(6+\frac{x}{20}\right)+$$
$$\left[z_{20}+\frac{z_{43}-z_{20}}{y_{43}-y_{20}}(y-y_{20})\right]M_3\left(5+\frac{x}{20}\right)+$$
$$\left[z_{21}+\frac{z_{44}-z_{21}}{y_{44}-y_{21}}(y-y_{21})\right]M_3\left(4+\frac{x}{20}\right)+$$
$$\left[z_{22}+\frac{z_{45}-z_{22}}{y_{45}-y_{22}}(y-y_{22})\right]M_3\left(3+\frac{x}{20}\right)+$$
$$\left[z_{23'}+\frac{z_{46}-z_{23'}}{y_{46}-y_{23'}}(y-y_{23'})\right]M_3\left(2+\frac{x}{20}\right)+$$
$$\left[2z_{23'}+2\frac{z_{46}-z_{23'}}{y_{46}-y_{23'}}(y-y_{23'}) - z_{22}-\frac{z_{45}-z_{22}}{y_{45}-y_{22}}(y-y_{22})\right]M_3\left(1+\frac{x}{20}\right)$$

By substituting y_i and $y_{23'}$ into the above equation, we obtain

$$z = S(x, y) = \left[2z_{17}+\frac{z_{40}-z_{17}}{20}y - z_{18}-\frac{z_{41}-z_{18}}{45}(y+2)\right]M_3\left(9+\frac{x}{20}\right)+$$
$$\left[z_{17}+\frac{z_{40}-z_{17}}{40}y\right]M_3\left(8+\frac{x}{20}\right)+$$
$$\left[z_{18}+\frac{z_{41}-z_{18}}{45}(y+2)\right]M_3\left(7+\frac{x}{20}\right)+$$
$$\left[z_{19}+\frac{z_{42}-z_{19}}{35}(y-2)\right]M_3\left(6+\frac{x}{20}\right)+$$
$$\left[z_{20}+\frac{z_{43}-z_{20}}{31}(y-3)\right]M_3\left(5+\frac{x}{20}\right)+$$
$$\left[z_{21}+\frac{z_{44}-z_{21}}{34}(y-4)\right]M_3\left(4+\frac{x}{20}\right)+$$
$$\left[z_{22}+\frac{z_{45}-z_{22}}{29}(y-8)\right]M_3\left(3+\frac{x}{20}\right)+$$
$$\left[z_{23'}+\frac{z_{46}-z_{23'}}{23}(y-9)\right]M_3\left(2+\frac{x}{20}\right)+$$
$$\left[2z_{23'}+2\frac{z_{46}-z_{23'}}{23}(y-9) - z_{22}-\frac{z_{45}-z_{22}}{29}(y-8)\right]M_3\left(1+\frac{x}{20}\right) \quad (10)$$

This is the mathematical model of concentration distributions of Mo, Ni and Fe in the δ-MoNi region. In eq. (10), let z_i and $z_{23'}$ be the concentration of Mo, Ni or Fe, then we obtain the concentration distribution functions of Mo, Ni and Fe in the δ-MoNi region respectively: $z = M(x, y)$, $z = N(x, y)$, $z = F(x, y)$.

For the P region, similar to the treatment of the δ-MoNi region, introducing assumed points 47′(−60, 30), 24′(−60, 9), 50′(20, 40) and 27′(20, 0) whose concentrations are

	Mo	Ni	Fe
$z_{47'}$	54.03	37.79	8.18
$z_{24'}$	48.06	39.81	12.13
$z_{50'}$	50.43	25.57	24.00

$z_{27'}$	49.26	33.19	17.55

then the mathematical model for concentration distributions is

$$
\begin{aligned}
z &= S(x, y) \\
&= \left[z_{24'} + \frac{z_{47'} - z_{24'}}{23}(y - 9)\right] M_3\left(3 + \frac{x}{20}\right) + \\
&\quad \left[z_{25} + \frac{z_{47} - z_{25}}{25}(y - 7)\right] M_3\left(2 + \frac{x}{20}\right) + \\
&\quad \left[z_{26} + \frac{z_{48} - z_{26}}{33}(y - 4)\right] M_3\left(1 + \frac{x}{20}\right) + \\
&\quad \left[z_{27} + \frac{z_{49} - z_{27}}{36} y\right] M_3\left(\frac{x}{20}\right) + \\
&\quad \left[z_{27'} + \frac{z_{50'} - z_{27'}}{40} y\right] M_3\left(-1 + \frac{x}{20}\right)
\end{aligned}
\tag{11}
$$

For the μ-Fe_7Mo_6 region, introducing assumed points 51′(0, 40), 51″(−20, 40), 28′(−20, 0) whose concentrations are

	Mo	Ni	Fe
$z_{51'}$	50.30	27.66	22.04
$z_{51''}$	53.65	31.19	15.16
$z_{28'}$	43.44	42.12	14.44

then the mathematical model for concentration distributions is

$$
\begin{aligned}
z &= S(x, y) \\
&= \left[z_{28'} + \frac{z_{51''} - z_{28'}}{40} y\right] M_3\left(1 + \frac{x}{20}\right) + \\
&\quad \left[z_{28} + \frac{z_{51'} - z_{28}}{40} y\right] M_3\left(\frac{x}{20}\right) + \\
&\quad \left[z_{29} + \frac{z_{52} - z_{29}}{48}(y + 4)\right] M_3\left(-1 + \frac{x}{20}\right) + \\
&\quad \left[z_{30} + \frac{z_{53} - z_{30}}{75}(y + 1)\right] M_3\left(-2 + \frac{x}{20}\right) + \\
&\quad \left[z_{31} + \frac{z_{54} - z_{31}}{112}(y + 20)\right] M_3\left(-3 + \frac{x}{20}\right) + \\
&\quad \left[z_{32} + \frac{z_{55} - z_{32}}{104}(y - 8)\right] M_3\left(-4 + \frac{x}{20}\right) + \\
&\quad \left[z_{33} + \frac{z_{56} - z_{33}}{88}(y - 37)\right] M_3\left(-5 + \frac{x}{20}\right) + \\
&\quad \left[z_{34} + \frac{z_{57} - z_{34}}{86}(y - 53)\right] M_3\left(-6 + \frac{x}{20}\right) + \\
&\quad \left[2z_{34} + \frac{z_{57} - z_{34}}{43}(y - 53) - \right. \\
&\quad \left. z_{33} - \frac{z_{56} - z_{33}}{88}(y - 37)\right] M_3\left(-7 + \frac{x}{20}\right)
\end{aligned}
\tag{12}
$$

For the *bcc* (Fe) region, introducing assumed points 37′(60, 8), 36″(60, −12) and 36′(80, −12) whose concentrations are

	Mo	Ni	Fe
$z_{37'}$	14.30	10.71	74.99
$z_{36''}$	0.43	7.71	81.86
$z_{36'}$	10.60	7.12	82.28

then the mathematical model for concentration distributions in the *bcc*(Fe) region is

$$
\begin{aligned}
z &= S(x, y) \\
&= \left[z_{36''} + \frac{z_{37'} - z_{36''}}{20}(y + 12)\right] M_3\left(-3 + \frac{x}{20}\right) + \\
&\quad \left[z_{36'} + \frac{z_{37} - z_{36'}}{20}(y + 12)\right] M_3\left(-4 + \frac{x}{20}\right) + \\
&\quad \left[z_{36} + \frac{z_{38} - z_{36}}{49}(y + 12)\right] M_3\left(-5 + \frac{x}{20}\right) + \\
&\quad \left[z_{35} + \frac{z_{39} - z_{35}}{89}(y + 36)\right] M_3\left(-6 + \frac{x}{20}\right) + \\
&\quad \left\{\left[2z_{35} + \frac{z_{39} - z_{35}}{44.5}(y + 36)\right] - \right. \\
&\quad \left. \left[z_{36} + \frac{z_{38} - z_{36}}{49}(y + 12)\right]\right\} M_3\left(-7 + \frac{x}{20}\right)
\end{aligned}
\tag{13}
$$

For the *bcc*(Mo) region, the mathematical model for concentration distributions is

$$
\begin{aligned}
z &= S(x, y) \\
&= \left[2z_{58} + \frac{z_{66} - z_{58}}{70}(y - 40) - \right. \\
&\quad \left. z_{59} - \frac{z_{67} - z_{59}}{143}(y - 37)\right] M_3\left(5 + \frac{x}{40}\right) + \\
&\quad \left[z_{58} + \frac{z_{66} - z_{58}}{140}(y - 40)\right] M_3\left(4 + \frac{x}{40}\right) + \\
&\quad \left[z_{59} + \frac{z_{67} - z_{59}}{143}(y - 37)\right] M_3\left(3 + \frac{x}{40}\right) + \\
&\quad \left[z_{60} + \frac{z_{68} - z_{60}}{142}(y - 38)\right] M_3\left(2 + \frac{x}{40}\right) + \\
&\quad \left[z_{61} + \frac{z_{69} - z_{61}}{148}(y - 32)\right] M_3\left(1 + \frac{x}{40}\right) + \\
&\quad \left[z_{62} + \frac{z_{70} - z_{62}}{144}(y - 36)\right] M_3\left(\frac{x}{40}\right) + \\
&\quad \left[z_{63} + \frac{z_{70} - z_{63}}{116}(y - 64)\right] M_3\left(-1 + \frac{x}{40}\right) + \\
&\quad \left[z_{64} + \frac{z_{72} - z_{64}}{116}(y - 112)\right] M_3\left(-2 + \frac{x}{40}\right) + \\
&\quad \left[z_{65} + \frac{z_{73} - z_{65}}{41}(y - 139)\right] M_3\left(-3 + \frac{x}{40}\right) + \\
&\quad \left[2z_{65} + \frac{z_{73} - z_{65}}{20.5}(y - 139) - \right. \\
&\quad \left. z_{64} - \frac{z_{72} - z_{64}}{68}(y - 112)\right] M_3\left(-4 + \frac{x}{40}\right)
\end{aligned}
\tag{14}
$$

For the *fcc* region, the mathematical model for concentration distributions is

$$z = S(x, y)$$

$$
\begin{aligned}
&= \{[2z_1 + \frac{z_9 - z_1}{40}(y + 80)] - \\
&[z_2 + \frac{z_{10} - z_2}{82}(y + 80)]\} M_3(5 + \frac{x}{40}) + \\
&[z_1 + \frac{z_9 - z_1}{80}(y + 80)] M_3(4 + \frac{x}{40}) + \\
&[z_2 + \frac{z_{10} - z_2}{82}(y + 80)] M_3(3 + \frac{x}{40}) + \\
&[z_3 + \frac{z_{11} - z_3}{84}(y + 80)] M_3(2 + \frac{x}{40}) + \\
&[z_4 + \frac{z_{12} - z_4}{87}(y + 80)] M_3(1 + \frac{x}{40}) + \\
&[z_5 + \frac{z_{13} - z_5}{80}(y + 80)] M_3(\frac{x}{40}) + \\
&[z_6 + \frac{z_{14} - z_6}{69}(y + 80)] M_3(-1 + \frac{x}{40}) + \\
&[z_7 + \frac{z_{15} - z_7}{88}(y + 80)] M_3(-2 + \frac{x}{40}) + \\
&[z_8 + \frac{z_{16} - z_8}{44}(y + 80)] M_3(-3 + \frac{x}{40}) + \\
&[2z_8 + \frac{z_{16} - z_8}{22}(y + 80) - \\
&z_7 - \frac{z_{15} - z_7}{88}(y + 80)] M_3(-4 + \frac{x}{40}) \quad (15)
\end{aligned}
$$

4.2 Mo-Ni-Co ternary system

Similar to the treatment of the Mo-Ni-Fe system in Fig. 1, we obtain the mathematical models of concentration distributions of Mo, Ni and Co in the Mo-Ni-Co system as shown in Fig. 2.

For the δ-MoNi region, introducing assumed point 33′ (0, 0) whose concentration $z_{33'}$ is: Mo, 47.17; Ni, 34.13; Co, 18.70. Then the mathematical model for concentration distributions is

$$
\begin{aligned}
z = S(x, y) &= [2z_{33'} + \frac{z_{39} - z_{33'}}{20} y - \\
&- z_{33} - \frac{z_{40} - z_{33}}{32} y] M_3(1 + \frac{x}{40}) + \\
&[z_{33'} + \frac{z_{39} - z_{33'}}{140} y] M_3(\frac{x}{40}) + \\
&[z_{33} + \frac{z_{40} - z_{33}}{32} y] M_3(-1 + \frac{x}{40}) + \\
&[z_{27} + \frac{z_{41} - z_{27}}{49}(y + 25)] M_3(-2 + \frac{x}{40}) + \\
&[z_{28} + \frac{z_{42} - z_{28}}{46}(y + 24)] M_3(-3 + \frac{x}{40}) + \\
&[z_{29} + \frac{z_{43} - z_{29}}{39}(y + 19)] M_3(-4 + \frac{x}{40}) + \\
&[z_{30} + \frac{z_{44} - z_{30}}{31}(y + 14)] M_3(-5 + \frac{x}{40}) + \\
&[z_{31} + \frac{z_{45} - z_{31}}{37}(y + 20)] M_3(-6 + \frac{x}{40}) + \\
&\{[2z_{31} + \frac{z_{45} - z_{31}}{18.5}(y + 20)] - \\
&[z_{30} + \frac{z_{44} - z_{30}}{31}(y + 14)]\} M_3(-7 + \frac{x}{40})
\end{aligned}
$$

(16)

For the μ-Co_7Mo_6 region, introducing assumed points 32′ (80, −13) and 25′ (80, −24) whose concentrations are

	Mo	Ni	Fe
$z_{32'}$	46.90	33.15	19.95
$z_{25'}$	48.20	38.78	13.02

then the mathematical model for concentration distributions is

$$
\begin{aligned}
z = S(x, y) &= [2z_{19} + \frac{z_{34} - z_{19}}{64}(y + 75) - \\
&z_{20} - \frac{z_{35} - z_{20}}{118}(y + 67)] M_3(5 + \frac{x}{40}) + \\
&[z_{19} + \frac{z_{34} - z_{19}}{128}(y + 75)] M_3(4 + \frac{x}{40}) + \\
&[z_{20} + \frac{z_{35} - z_{20}}{118}(y + 67)] M_3(3 + \frac{x}{40}) + \\
&[z_{21} + \frac{z_{36} - z_{21}}{109}(y + 61)] M_3(2 + \frac{x}{40}) + \\
&[z_{22} + \frac{z_{37} - z_{22}}{90}(y + 47)] M_3(1 + \frac{x}{40}) + \\
&[z_{23} + \frac{z_{38} - z_{23}}{77}(y + 37)] M_3(\frac{x}{40}) + \\
&[z_{24} + \frac{z_{32} - z_{24}}{8}(y + 21)] M_3(-1 + \frac{x}{40}) + \\
&[z_{25'} + \frac{z_{32'} - z_{25'}}{11}(y + 24)] M_3(-2 + \frac{x}{40})
\end{aligned}
$$

(17)

For the *bcc*(Mo) region, the mathematical model for concentration distributions is

$$
\begin{aligned}
z &= S(x, y) \\
&= [z_{46} + \frac{z_{57} - z_{46}}{127}(y - 53)] M_3(2 + \frac{x}{80}) + \\
&[z_{48} + \frac{z_{58} - z_{48}}{132}(y - 48)] M_3(1 + \frac{x}{80}) + \\
&[z_{50} + \frac{z_{59} - z_{50}}{140}(y - 40)] M_3(\frac{x}{80}) + \\
&[z_{52} + \frac{z_{60} - z_{52}}{156}(y - 24)] M_3(-1 + \frac{x}{80}) + \\
&[z_{54} + \frac{z_{61} - z_{54}}{160}(y - 20)] M_3(-2 + \frac{x}{80}) + \\
&[z_{56} + \frac{z_{62} - z_{56}}{163}(y - 17)] M_3(-3 + \frac{x}{80}) + \\
&[2z_{46} + \frac{z_{57} - z_{46}}{63.5}(y - 53) -
\end{aligned}
$$

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state.

(2) The fairly perfect *nn* order and *nnn* order exist in the air-quenched martensite of Cu-18Zn-14Al alloy whose atomic distribution on the basic plane is as follows. Ⅰ —(14/25) Al+ (11/25) Cu, Ⅱ is Cu, Ⅲ is (18/25) Zn+ (7/25) Cu, as shown in Fig. 2(b).

(3) The martensite stabilization still occurred in the air-quenched alloy. The function is limited to suppress the martensite stabilization through enhancing order degree of the alloy.

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$$
\begin{aligned}
& z_{48}-\frac{z_{58}-z_{48}}{132}(y-48)]M_3(3+\frac{x}{80})+ \\
& [2z_{56}+\frac{z_{62}-z_{56}}{81.5}(y-17)- \\
& z_{54}-\frac{z_{61}-z_{54}}{160}(y-20)]M_3(-4+\frac{x}{80})
\end{aligned} \tag{18}
$$

For the *fcc* region, the mathematical model for concentration distributions is

$$
\begin{aligned}
z = & \ S(x, y) \\
= & \ [2z_1+\frac{z_7-z_1}{42.5}(y+160)- \\
& z_2-\frac{z_9-z_2}{99}(y+160)]M_3(3+\frac{x}{80})+ \\
& [z_1+\frac{z_7-z_1}{85}(y+160)]M_3(2+\frac{x}{80})+ \\
& [z_2+\frac{z_9-z_2}{99}(y+160)]M_3(1+\frac{x}{80})+ \\
& [z_3+\frac{z_{11}-z_3}{123}(y+160)]M_3(\frac{x}{80})+ \\
& [z_4+\frac{z_{14}-z_4}{135}(y+160)]M_3(-1+\frac{x}{80})+ \\
& [z_5+\frac{z_{16}-z_5}{141}(y+160)]M_3(-2+\frac{x}{80})+ \\
& [z_6+\frac{z_{18}-z_6}{140}(y+160)]M_3(-3+\frac{x}{80})+ \\
& \{[2z_6+\frac{z_{18}-z_6}{70}(y+160)]- \\
& [z_5+\frac{z_{16}-z_5}{141}(y+160)]\}M_3(-4+\frac{x}{80})
\end{aligned} \tag{19}
$$

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