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# Characteristic atom sequences of Nb−Mo alloys system in BCC structure and properties of disordered alloys

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**Abstract:** Comprehensively considering energy, volume and electronic structure of alloys, the ninth equation was determined as the interaction function of Nb−Mo alloys system in BCC structure on the basis of idea of systematic science of alloys, experimental lattice constants and heats of formation of disordered $Nb_{(1-x)}Mo_x$ alloys. The structural parameters and properties of Nb and Mo characteristic atoms sequences and corresponding characteristic crystals sequences were determined in Nb−Mo alloys system. The electronic structure and physical properties of disordered $Nb_{(1-x)}Mo_x$ alloys system were calculated according to concentration of characteristic atoms of disordered alloys. The change trend of physical properties is the same as that of electronic structure.
**Key words:** Nb−Mo alloys system; characteristic atom sequences; disordered alloys; properties

## 1 Introduction

The target of material science development is to continuously design and develop new materials to meet modernization and future needs. To develop material design by multi-structure levels and various properties, materials science should be systematic. After nearly thirty years of efforts, XIE et al [1−12] had established the framework of systematic science of alloys on the basis of energy band theory, valence bond theory and statistical thermodynamics. The core is the theory of the characteristic crystals and points out direction of alloy design. The theory has been successfully applied to Ag−Cu alloys [1−4] and Au−Cu alloys [5−8] in FCC structure, Ti−Al alloys with coexistence of FCC and HCP structures [9−12].

However, there is little research on alloys in BCC structure by the theory. The purpose of the present work is to choose Nb−Mo alloys in BCC structure as research subject. Based on the experimental lattice constants, heats of formation of disordered $Nb_{(1-x)}Mo_x$ alloys and the theory of the characteristic crystals, comprehensively considering the energy, volume and electronic structure of alloys, the optimum equation was determined as the interaction function of Nb−Mo alloys system. The structural parameters and properties of Nb and Mo characteristic atoms sequences and corresponding characteristic crystals sequences in Nb−Mo alloys system were determined. According to the concentrations of the characteristic atoms, the structural parameters and properties of disordered $Nb_{(1-x)}Mo_x$ alloys were obtained. The framework of systematic science of alloys will be further developed and improved.

## 2 Models and laws

In the disordered solid solution, the concentrations of characteristic atoms are, respectively

$$\begin{cases} x_i^{\mathrm{A}} = C_I^i x_{\mathrm{A}}^{(I-i+1)} x_{\mathrm{B}}^i \\ x_i^{\mathrm{B}} = C_I^i x_{\mathrm{A}}^{(I-i)} x_{\mathrm{B}}^{(i+1)} \end{cases} \tag{1}$$

where $C_I^i$ is the combination factor $I!/[(I-i)!i!]$.

The average atomic energy of the alloys is

$$q = x_{\mathrm{A}}\left(\sum_{i=0}^{I} C_I^i x_{\mathrm{A}}^{(I-i)} x_{\mathrm{B}}^i q_i^{\mathrm{A}}\right) + x_{\mathrm{B}}\left(\sum_{i=0}^{I} C_I^i x_{\mathrm{A}}^{(I-i)} x_{\mathrm{B}}^i q_i^{\mathrm{B}}\right) \tag{2}$$

The average atomic energies of components are, respectively

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$$q_{\mathrm{A}}=\sum_{i=0}^{I}C_I^i x_{\mathrm{A}}^{(I-i)}x_{\mathrm{B}}^i q_i^{\mathrm{A}} \tag{3}$$

$$q_{\mathrm{B}}=\sum_{i=0}^{I}C_I^i x_{\mathrm{A}}^{(I-i)}x_{\mathrm{B}}^i q_i^{\mathrm{B}} \tag{4}$$

Substituting relations of property $q_i^{\mathrm{A}}$ of characteristic crystals of component A and $i$ into Eq. (4), three relations of average property $q_{\mathrm{A}}$ of component A with composition $x_{\mathrm{A}}$ can be obtained (the derivation is omitted here):

For type I,

$$q_{\mathrm{A}}=q_{\mathrm{A}}^0+x_{\mathrm{B}}(q_I^{\mathrm{A}}-q_{\mathrm{A}}^0); \tag{5}$$

For type II,

$$q_{\mathrm{A}}=q_{\mathrm{A}}^0+\{[x_{\mathrm{B}}+(I-1)x_{\mathrm{B}}^2]/I\}(q_I^A-q_{\mathrm{A}}^0) \tag{6}$$

For type III,

$$q_{\mathrm{A}}=q_{\mathrm{A}}^0+\{[Ix_{\mathrm{B}}+(I-1)x_{\mathrm{A}}x_{\mathrm{B}}]/I\}(q_I^{\mathrm{A}}-q_{\mathrm{A}}^0) \tag{7}$$

Similarly, three relations of average property $q_{\mathrm{B}}$ of component B with composition $x_{\mathrm{B}}$ can be obtained (the derivation is omitted here):

For type I,

$$q_{\mathrm{B}}=q_{\mathrm{B}}^0+x_{\mathrm{A}}(q_0^{\mathrm{B}}-q_{\mathrm{B}}^0); \tag{8}$$

For type II,

$$q_{\mathrm{B}}=q_{\mathrm{B}}^0+\{[x_{\mathrm{A}}+(I-1)x_{\mathrm{A}}^2]/I\}(q_0^{\mathrm{B}}-q_{\mathrm{B}}^0) \tag{9}$$

For type III,

$$q_{\mathrm{B}}=q_{\mathrm{B}}^0+\{[Ix_{\mathrm{A}}+(I-1)x_{\mathrm{A}}x_{\mathrm{B}}]/I\}(q_0^{\mathrm{B}}-q_{\mathrm{B}}^0) \tag{10}$$

Combining the above equations and substituting them into Eq. (2), nine equations of average atomic potential energy and average atomic volume of solid solution can be obtained(see Table 1). For alloys system in BCC structure, $I$=8.

### 2.1 Determination of cohesive energies of Nb and Mo characteristic crystals of Nb−Mo alloys system in BCC structure

The crystalline structure of pure metals Nb and Mo is the same as that of Nb−Mo solid solutions. $E_{\mathrm{c}0}^{\mathrm{Nb}}$ and $E_{\mathrm{c}I}^{\mathrm{Mo}}$ refer to cohesive energies of pure metals Nb and Mo, respectively. $E_{\mathrm{c}I}^{\mathrm{Nb}}$ and $E_{\mathrm{c}0}^{\mathrm{Mo}}$ are calculated by interaction equations of binary disordered alloys [13] from heats of formation [14] of $Nb_{(1-x)}Mo_x$ solid solutions with different compositions. The results are listed in Table 2.

If we only consider the energy of disordered $Nb_{(1-x)}Mo_x$ alloy system in BCC structure, not average energy of every characteristic crystal, nine interaction equations are feasible in Table 1. The cohesive energies of the terminal state characteristic crystals are different from various equations. The cohesive energies of characteristic crystals by nine equations are listed in Table 3.

**Table 1** Interaction equations of binary disordered alloys ($q$=$E$, $v$)

| No. | Interaction equation of binary disordered alloys |
|---|---|
| 1 | $q=x_{\mathrm{A}}q_0^{\mathrm{A}}+x_{\mathrm{B}}q_I^{\mathrm{B}}+x_{\mathrm{A}}x_{\mathrm{B}}[(q_I^{\mathrm{A}}-q_0^{\mathrm{A}})+(q_0^{\mathrm{B}}-q_I^{\mathrm{B}})]$ |
| 2 | $q=x_{\mathrm{A}}q_0^{\mathrm{A}}+x_{\mathrm{B}}q_I^{\mathrm{B}}+x_{\mathrm{A}}x_{\mathrm{B}}(q_I^{\mathrm{A}}-q_0^{\mathrm{A}})+\frac{(I-1)x_{\mathrm{A}}{}^2x_{\mathrm{B}}+x_{\mathrm{A}}x_{\mathrm{B}}}{I}(q_0^{\mathrm{B}}-q_I^{\mathrm{B}})$ |
| 3 | $q=x_{\mathrm{A}}q_0^{\mathrm{A}}+x_{\mathrm{B}}q_I^{\mathrm{B}}+x_{\mathrm{A}}x_{\mathrm{B}}(q_I^{\mathrm{A}}-q_0^{\mathrm{A}})+\frac{(I-1)x_{\mathrm{A}}x_{\mathrm{B}}{}^2+Ix_{\mathrm{A}}x_{\mathrm{B}}}{I}(q_0^{\mathrm{B}}-q_{\mathrm{I}}^{\mathrm{B}})$ |
| 4 | $q=x_{\mathrm{A}}q_0^{\mathrm{A}}+x_{\mathrm{B}}q_I^{\mathrm{B}}+\frac{(I-1)x_{\mathrm{A}}x_{\mathrm{B}}^2+x_{\mathrm{A}}x_{\mathrm{B}}}{I}\cdot(q_I^{\mathrm{A}}-q_0^{\mathrm{A}})+x_{\mathrm{A}}x_{\mathrm{B}}(q_0^{\mathrm{B}}-q_I^{\mathrm{B}})$ |
| 5 | $q=x_{\mathrm{A}}q_0^{\mathrm{A}}+x_{\mathrm{B}}q_I^{\mathrm{B}}+\frac{(I-1)x_{\mathrm{A}}x_{\mathrm{B}}^2+x_{\mathrm{A}}x_{\mathrm{B}}}{I}(q_I^{\mathrm{A}}-q_0^{\mathrm{A}})+\frac{(I-1)x_{\mathrm{A}}^2x_{\mathrm{B}}+x_{\mathrm{A}}x_{\mathrm{B}}}{I}(q_0^{\mathrm{B}}-q_I^{\mathrm{B}})$ |
| 6 | $q=x_{\mathrm{A}}q_0^{\mathrm{A}}+x_{\mathrm{B}}q_I^{\mathrm{B}}+\frac{(I-1)x_{\mathrm{A}}x_{\mathrm{B}}^2+x_{\mathrm{A}}x_{\mathrm{B}}}{I}(q_I^{\mathrm{A}}-q_0^{\mathrm{A}})+\frac{(I-1)x_{\mathrm{A}}^2x_{\mathrm{B}}+Ix_{\mathrm{A}}x_{\mathrm{B}}}{I}(q_0^{\mathrm{B}}-q_I^{\mathrm{B}})$ |
| 7 | $q=x_{\mathrm{A}}q_0^{\mathrm{A}}+x_{\mathrm{B}}q_I^{\mathrm{B}}+\frac{(I-1)x_{\mathrm{A}}^2x_{\mathrm{B}}+Ix_{\mathrm{A}}x_{\mathrm{B}}}{I}\cdot(q_I^{\mathrm{A}}-q_0^{\mathrm{A}})+x_{\mathrm{A}}x_{\mathrm{B}}(q_0^{\mathrm{B}}-q_I^{\mathrm{B}})$ |
| 8 | $q=x_{\mathrm{A}}q_0^{\mathrm{A}}+x_{\mathrm{B}}q_I^{\mathrm{B}}+\frac{(I-1)x_{\mathrm{A}}^2x_{\mathrm{B}}+Ix_{\mathrm{A}}x_{\mathrm{B}}}{I}(q_I^{\mathrm{A}}-q_0^{\mathrm{A}})+\frac{(I-1)x_{\mathrm{A}}^2x_{\mathrm{B}}+x_{\mathrm{A}}x_{\mathrm{B}}}{I}(q_0^{\mathrm{B}}-q_I^{\mathrm{B}})$ |
| 9 | $q=x_{\mathrm{A}}q_0^{\mathrm{A}}+x_{\mathrm{B}}q_I^{\mathrm{B}}+\frac{(I-1)x_{\mathrm{A}}^2x_{\mathrm{B}}+Ix_{\mathrm{A}}x_{\mathrm{B}}}{I}(q_I^{\mathrm{A}}-q_0^{\mathrm{A}})+\frac{(I-1)x_{\mathrm{A}}x_{\mathrm{B}}^2+Ix_{\mathrm{A}}x_{\mathrm{B}}}{I}(q_0^{\mathrm{B}}-q_I^{\mathrm{B}})$ |

**Table 2** Terminal and primary values of cohesive energies of Nb and Mo characteristic crystals of Nb−Mo alloys system

| No. | $E_{\mathrm{c}0}^{\mathrm{Nb}}$ / (kJ·mol$^{-1}$) | $E_{\mathrm{c}I}^{\mathrm{Nb}}$ / (kJ·mol$^{-1}$) | $E_{\mathrm{c}I}^{\mathrm{Mo}}$ / (kJ·mol$^{-1}$) | $E_{\mathrm{c}0}^{\mathrm{Mo}}$ / (kJ·mol$^{-1}$) |
|---|---|---|---|---|
| 1 | 730.00 | 728.10 | 658.00 | 728.10 |
| 2 | 730.00 | 787.66 | 658.00 | 676.75 |
| 3 | 730.00 | 825.15 | 658.00 | 639.25 |
| 4 | 730.00 | 711.25 | 658.00 | 736.75 |
| 5 | 730.00 | 781.25 | 658.00 | 728.00 |
| 6 | 730.00 | 621.26 | 658.00 | 748.00 |
| 7 | 730.00 | 748.75 | 658.00 | 699.26 |
| 8 | 730.00 | 795.89 | 658.00 | 610.85 |
| 9 | 730.00 | 763.10 | 658.00 | 672.35 |

**Table 3** Cohesive energies of characteristic crystals Nb and Mo of Nb−Mo alloys system by nine interaction equations

| Characteristic crystal | $i$ | Cohesive energy/(kJ·mol$^{-1}$) | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 |
| Nb | 1 | 730.00 | 729.76 | 729.53 | 729.29 | 729.05 | 728.81 | 728.58 | 728.34 | 728.10 |
| | 2 | 730.00 | 737.21 | 744.41 | 751.62 | 758.83 | 766.04 | 773.24 | 780.45 | 787.66 |
| | 3 | 730.00 | 741.89 | 753.79 | 765.68 | 777.57 | 789.47 | 801.36 | 813.26 | 825.15 |
| | 4 | 730.00 | 729.71 | 728.83 | 727.36 | 725.31 | 722.68 | 719.46 | 715.65 | 711.25 |
| | 5 | 730.00 | 730.80 | 733.20 | 737.21 | 742.81 | 750.02 | 758.83 | 769.24 | 781.25 |
| | 6 | 730.00 | 728.30 | 723.20 | 714.71 | 702.81 | 687.52 | 668.83 | 646.74 | 621.26 |
| | 7 | 730.00 | 734.39 | 738.20 | 741.42 | 744.06 | 746.11 | 747.57 | 748.45 | 748.75 |
| | 8 | 730.00 | 745.44 | 758.83 | 770.15 | 779.42 | 786.63 | 791.78 | 794.87 | 795.89 |
| | 9 | 730.00 | 737.76 | 744.48 | 750.17 | 754.82 | 758.44 | 761.03 | 762.58 | 763.10 |
| Mo | 1 | 728.10 | 719.34 | 710.58 | 701.81 | 693.05 | 684.29 | 675.53 | 666.76 | 658.00 |
| | 2 | 676.75 | 672.35 | 668.54 | 665.32 | 662.69 | 660.64 | 659.17 | 658.29 | 658.00 |
| | 3 | 639.25 | 639.55 | 640.43 | 641.89 | 643.94 | 646.58 | 649.80 | 653.61 | 658.00 |
| | 4 | 736.75 | 726.90 | 717.06 | 707.22 | 697.37 | 687.53 | 677.69 | 667.84 | 658.00 |
| | 5 | 728.00 | 711.59 | 697.37 | 685.34 | 675.50 | 667.84 | 662.37 | 659.09 | 658.00 |
| | 6 | 748.00 | 746.59 | 742.37 | 735.34 | 725.50 | 712.84 | 697.37 | 679.09 | 658.00 |
| | 7 | 699.26 | 694.10 | 688.94 | 683.78 | 678.63 | 673.47 | 668.31 | 663.16 | 658.00 |
| | 8 | 610.85 | 621.90 | 631.48 | 639.58 | 646.21 | 651.37 | 655.05 | 657.26 | 658.00 |
| | 9 | 672.35 | 672.13 | 671.45 | 670.33 | 668.76 | 666.74 | 664.28 | 661.36 | 658.00 |

### 2.2 Determination of lattice constants of characteristic crystals Nb and Mo of Nb−Mo alloys system in BCC structure

The crystalline structure of pure metals Nb and Mo is also the same as that of Nb−Mo solid solutions. $v_0^{\mathrm{Nb}}$ and $v_I^{\mathrm{Mo}}$ refer to atomic volumes of pure metals Nb and Mo, respectively. $v_I^{\mathrm{Nb}}$ and $v_0^{\mathrm{Mo}}$ are calculated by volume interaction equations of binary disordered alloys from experimental lattice constants [15] of $\mathrm{Nb}_{(1-x)}\mathrm{Mo}_x$ solid solutions with different compositions. The results are listed in Table 4.

If we only consider the atomic volumes of disordered $\mathrm{Nb}_{(1-x)}\mathrm{Mo}_x$ alloys system in BCC structure, not average atomic volumes of every characteristic crystal, nine interaction equations are also feasible in Table 1. The atomic volumes of the terminal state characteristic crystals are different from various equations. The lattice constants of Nb and Mo characteristic crystals by nine equations are listed in Table 5.

The research on energy and volume interaction equations of alloys indicates that primary values are the same by different interaction equations. But cohesive energies of different characteristic crystals have great differences by different interaction equations. Therefore, every interaction equation describes a specific interaction essence of Nb and Mo atoms in the theory of characteristic crystals and reflects microscope essence of solid solution. It is incorrect that the interaction equations are chosen only from alloy energy as a function of composition. Only considering the relationship among energy, volume, atomic state of alloy, the correct interaction equation can be chosen. The ninth equation is determined as interaction equation of disordered $\mathrm{Nb}_{(1-x)}\mathrm{Mo}_x$ alloys by systematic analysis of properties of characteristic crystals in Tables 3 and 5.

$$E_{\mathrm{c}} = x_{\mathrm{Nb}}E_{\mathrm{c}0}^{\mathrm{Nb}} + x_{\mathrm{Mo}}E_{\mathrm{c}I}^{\mathrm{Mo}} + \frac{(I-1)x_{\mathrm{Nb}}^2x_{\mathrm{Mo}} + Ix_{\mathrm{Nb}}x_{\mathrm{Mo}}}{I}\cdot (E_{\mathrm{c}I}^{\mathrm{Nb}} - E_{\mathrm{c}0}^{\mathrm{Nb}}) + \frac{(I-1)x_{\mathrm{Nb}}x_{\mathrm{Mo}}^2 + Ix_{\mathrm{Nb}}x_{\mathrm{Mo}}}{I}(E_{\mathrm{c}0}^{\mathrm{Mo}} - E_{\mathrm{c}I}^{\mathrm{Mo}}) \tag{11}$$

**Table 4** Terminal and primary values of volume of Nb and Mo characteristic crystals of Nb−Mo alloys system

| No. | $v_0^{\mathrm{Nb}}$ / $10^{-3}$ nm$^3$ | $v_I^{\mathrm{Nb}}$ / $10^{-3}$ nm$^3$ | $v_I^{\mathrm{Mo}}$ / $10^{-3}$ nm$^3$ | $v_0^{\mathrm{Mo}}$ / $10^{-3}$ nm$^3$ |
|---|---|---|---|---|
| 1 | 17.9750 | 16.2633 | 15.5893 | 16.2633 |
| 2 | 17.9750 | 17.0198 | 15.5893 | 15.4200 |
| 3 | 17.9750 | 16.6813 | 15.5893 | 15.7585 |
| 4 | 17.9750 | 18.1443 | 15.5893 | 14.4437 |
| 5 | 17.9750 | 17.1260 | 15.5893 | 14.5709 |
| 6 | 17.9750 | 19.4536 | 15.5893 | 14.2800 |
| 7 | 17.9750 | 17.8058 | 15.5893 | 14.7822 |
| 8 | 17.9750 | 16.8834 | 15.5893 | 16.5117 |
| 9 | 17.9750 | 17.5250 | 15.5893 | 15.3085 |

**Table 5** Lattice constants of Nb and Mo characteristic crystals of Nb−Mo alloys system by nine interaction equations

| Characteristic crystal | $i$ | Lattice constant/$10^{-1}$nm | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 |
| Nb | 1 | 3.3004 | 3.2873 | 3.2740 | 3.2606 | 3.2472 | 3.2336 | 3.2199 | 3.2061 | 3.1921 |
| | 2 | 3.3004 | 3.2931 | 3.2857 | 3.2783 | 3.2709 | 3.2634 | 3.2560 | 3.2484 | 3.2409 |
| | 3 | 3.3004 | 3.2905 | 3.2805 | 3.2704 | 3.2603 | 3.2502 | 3.2399 | 3.2296 | 3.2192 |
| | 4 | 3.3004 | 3.3006 | 3.3010 | 3.3019 | 3.3030 | 3.3044 | 3.3062 | 3.3083 | 3.3107 |
| | 5 | 3.3004 | 3.2996 | 3.2971 | 3.2931 | 3.2874 | 3.2800 | 3.2709 | 3.2601 | 3.2476 |
| | 6 | 3.3004 | 3.3018 | 3.3060 | 3.3131 | 3.3229 | 3.3354 | 3.3505 | 3.3683 | 3.3885 |
| | 7 | 3.3004 | 3.2980 | 3.2959 | 3.2941 | 3.2926 | 3.2915 | 3.2907 | 3.2902 | 3.2900 |
| | 8 | 3.3004 | 3.2847 | 3.2709 | 3.2592 | 3.2495 | 3.2420 | 3.2365 | 3.2333 | 3.2322 |
| | 9 | 3.3004 | 3.2939 | 3.2883 | 3.2835 | 3.2796 | 3.2766 | 3.2744 | 3.2731 | 3.2726 |
| Mo | 1 | 3.1921 | 3.1866 | 3.1811 | 3.1755 | 3.1699 | 3.1643 | 3.1587 | 3.1531 | 3.1474 |
| | 2 | 3.1360 | 3.1387 | 3.1410 | 3.1429 | 3.1445 | 3.1458 | 3.1467 | 3.1472 | 3.1474 |
| | 3 | 3.1587 | 3.1586 | 3.1580 | 3.1572 | 3.1559 | 3.1543 | 3.1524 | 3.1501 | 3.1474 |
| | 4 | 3.0683 | 3.0784 | 3.0885 | 3.0985 | 3.1084 | 3.1182 | 3.1280 | 3.1377 | 3.1474 |
| | 5 | 3.0773 | 3.0940 | 3.1084 | 3.1204 | 3.1302 | 3.1377 | 3.1431 | 3.1463 | 3.1474 |
| | 6 | 3.0567 | 3.0582 | 3.0625 | 3.0698 | 3.0799 | 3.0928 | 3.1084 | 3.1266 | 3.1474 |
| | 7 | 3.0921 | 3.0991 | 3.1061 | 3.1131 | 3.1200 | 3.1269 | 3.1338 | 3.1406 | 3.1474 |
| | 8 | 3.2083 | 3.1942 | 3.1819 | 3.1715 | 3.1628 | 3.1561 | 3.1513 | 3.1484 | 3.1474 |
| | 9 | 3.1284 | 3.1287 | 3.1296 | 3.1311 | 3.1332 | 3.1358 | 3.1391 | 3.1430 | 3.1474 |

where $E_{c0}^{Nb}$ =730 kJ/mol, $E_{cI}^{Mo}$ =658 kJ/mol, $E_{cI}^{Nb}$ = 763.10 kJ/mol, $E_{c0}^{Mo}$ =672.35 kJ/mol, $I$=8.

$$v = x_{Nb}v_0^{Nb} + x_{Mo}v_I^{Mo} + \frac{(I-1)x_{Nb}^2x_{Mo} + Ix_{Nb}x_{Mo}}{I}\cdot$$
$$(v_I^{Nb} - v_0^{Nb}) + \frac{(I-1)x_{Nb}x_{Mo}^2 + Ix_{Nb}x_{Mo}}{I}(v_0^{Mo} - v_I^{Mo}) \quad (12)$$

where $v_0^{Nb}$ =0.0179750 nm$^3$, $v_I^{Mo}$ =0.0155893 nm$^3$, $v_I^{Nb}$ =0.0175250 nm$^3$, $v_0^{Mo}$ =0.0153085 nm$^3$, and $I$=8.

## 3 Nb and Mo characteristic atom sequences and characteristic crystal sequences of Nb−Mo alloys system in BCC structure

Structural parameters and properties of Nb and Mo characteristic atoms sequences and corresponding characteristic crystals sequences in Nb−Mo alloys system by experimental cohesive energies and lattice constants obtained by the ninth equation are listed in Tables 6 and 7. In the tables, $d_c$, $s_c$ and $p_c$ are the number of covalent electrons in s，p, and d orbits; $e_c$ is the summation of covalent electrons; $e_f$ is the summation of free electrons; $e_n$ is the summation of non-bonded electrons; $R$ is the single radius; $r_i$ is the bond length of the $i$th neighbor bond; $n_i$ is the number of the $i$th neighbor bond; $E_1$ is the bond energy in the nearest neighbor bond; $E_c$ is cohesive energy.

## 4 Properties of disordered $Nb_{(1-x)}Mo_x$ alloys system in BCC structure

The properties of alloys are described by average properties of components. The properties of disordered alloys are obtained by additive law of characteristic crystals. Therefore, electronic structure and properties of disordered $Nb_{(1-x)}Mo_x$ alloys system as a function of composition $x_{Mo}$ are listed in Table 8.

The electronic structures and properties of disordered $Nb_{(1-x)}Mo_x$ alloys system as function of composition $x_{Mo}$ are shown in Figs. 1−3. As can be seen in Fig. 1, the number of covalent electrons $e_c$ increases and the number of free electron $e_f$ decreases with the concentration of Mo increasing. This is consistent with the cohesive energy. Figure 2 illustrates the relationship between bond length and composition. Single bond radius reduces with increasing the concentration of Mo. Figure 3 shows the relationship between the nearest neighbor bond length and bond energy. Bond length becomes short with increasing the concentration of Mo, electron pairs increase and bond energy decreases, and the change trend is very similar to that of electronic structure.

**Table 6** Structural parameters and properties of Nb characteristic atom sequences and corresponding characteristic crystal sequences in Nb−Mo alloys system

| $i$ | $d_c$ | $s_c$ | $p_c$ | $e_c$ | $e_f$ | $e_n$ | $R/10^{-1}$nm | $r_1/10^{-1}$nm | $r_2/10^{-1}$nm | $r_3/10^{-1}$nm | $n_1$ | $n_2$ | $n_3$ | $E_1$/(kJ·mol$^{-1}$) | $E_c$/(kJ·mol$^{-1}$) |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | 2.0929 | 0.4220 | 1.2600 | 3.7749 | 1.2251 | 0 | 1.3143 | 2.8582 | 3.3004 | 4.6675 | 0.4143 | 0.0759 | 0.0004 | 611.0474 | 729.9994 |
| 1 | 2.1017 | 0.4240 | 1.2660 | 3.7917 | 1.2083 | 0 | 1.3120 | 2.8526 | 3.2939 | 4.6583 | 0.4160 | 0.0765 | 0.0004 | 618.3618 | 737.7561 |
| 2 | 2.1116 | 0.4240 | 1.2700 | 3.8056 | 1.1944 | 0 | 1.3100 | 2.8478 | 3.2883 | 4.6504 | 0.4174 | 0.0770 | 0.0004 | 624.6575 | 744.4792 |
| 3 | 2.1184 | 0.4260 | 1.2760 | 3.8204 | 1.1796 | 0 | 1.3084 | 2.8436 | 3.2835 | 4.6436 | 0.4188 | 0.0774 | 0.0004 | 630.1646 | 750.1672 |
| 4 | 2.1239 | 0.4280 | 1.2800 | 3.8319 | 1.1681 | 0 | 1.3071 | 2.8402 | 3.2796 | 4.6381 | 0.4200 | 0.0778 | 0.0004 | 634.6363 | 754.8210 |
| 5 | 2.1301 | 0.4280 | 1.2820 | 3.8401 | 1.1599 | 0 | 1.3060 | 2.8376 | 3.2766 | 4.6338 | 0.4208 | 0.0781 | 0.0004 | 638.0674 | 758.4412 |
| 6 | 2.1328 | 0.4300 | 1.2840 | 3.8468 | 1.1532 | 0 | 1.3053 | 2.8357 | 3.2744 | 4.6307 | 0.4215 | 0.0783 | 0.0004 | 640.5722 | 761.0265 |
| 7 | 2.1341 | 0.4300 | 1.2860 | 3.8501 | 1.1499 | 0 | 1.3048 | 2.8346 | 3.2731 | 4.6288 | 0.4218 | 0.0784 | 0.0004 | 642.0285 | 762.5778 |
| 8 | 2.1358 | 0.4300 | 1.2860 | 3.8518 | 1.1482 | 0 | 1.3047 | 2.8342 | 3.2726 | 4.6282 | 0.4220 | 0.0784 | 0.0004 | 642.5542 | 763.0951 |

**Table 7** Structural parameters and properties of Mo characteristic atom sequences and corresponding characteristic crystal sequences in Nb−Mo alloys system

| $i$ | $d_c$ | $s_c$ | $p_c$ | $e_c$ | $e_f$ | $e_n$ | $R/10^{-1}$nm | $r_1/10^{-1}$nm | $r_2/10^{-1}$nm | $r_3/10^{-1}$nm | $n_1$ | $n_2$ | $n_3$ | $E_1$/(kJ·mol$^{-1}$) | $E_c$/(kJ·mol$^{-1}$) |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | 2.7436 | 0.5520 | 1.6500 | 4.9456 | 1.0544 | 0 | 1.2735 | 2.7093 | 3.1284 | 4.4242 | 0.5365 | 0.1074 | 0.0007 | 573.8869 | 672.3494 |
| 1 | 2.7424 | 0.5520 | 1.6500 | 4.9444 | 1.0556 | 0 | 1.2736 | 2.7095 | 3.1287 | 4.4246 | 0.5364 | 0.1074 | 0.0007 | 573.6649 | 672.1252 |
| 2 | 2.7409 | 0.5500 | 1.6480 | 4.9389 | 1.0611 | 0 | 1.2739 | 2.7103 | 3.1296 | 4.4259 | 0.5358 | 0.1072 | 0.0007 | 572.9346 | 671.4528 |
| 3 | 2.7368 | 0.5500 | 1.6480 | 4.9348 | 1.0652 | 0 | 1.2744 | 2.7116 | 3.1311 | 4.4280 | 0.5355 | 0.1070 | 0.0007 | 571.8905 | 670.3315 |
| 4 | 2.7325 | 0.5500 | 1.6440 | 4.9265 | 1.0735 | 0 | 1.2751 | 2.7134 | 3.1332 | 4.4310 | 0.5346 | 0.1068 | 0.0007 | 570.3388 | 668.7620 |
| 5 | 2.7277 | 0.5480 | 1.6420 | 4.9177 | 1.0823 | 0 | 1.2761 | 2.7157 | 3.1358 | 4.4348 | 0.5338 | 0.1065 | 0.0007 | 568.4105 | 666.7441 |
| 6 | 2.7208 | 0.5480 | 1.6380 | 4.9068 | 1.0932 | 0 | 1.2772 | 2.7186 | 3.1391 | 4.4394 | 0.5327 | 0.1061 | 0.0007 | 566.0415 | 664.2776 |
| 7 | 2.7137 | 0.5460 | 1.6320 | 4.8917 | 1.1083 | 0 | 1.2785 | 2.7219 | 3.1430 | 4.4448 | 0.5312 | 0.1056 | 0.0007 | 563.1677 | 661.3629 |
| 8 | 2.7045 | 0.5440 | 1.6280 | 4.8765 | 1.1235 | 0 | 1.2801 | 2.7257 | 3.1474 | 4.4511 | 0.5297 | 0.1050 | 0.0007 | 559.9220 | 657.9997 |

**Table 8** Electronic structure and properties of disordered $Nb_{(1-x)}Mo_x$ alloys system as function of composition $x_{Mo}$

| $x_{Mo}$ | $d_c$ | $s_c$ | $p_c$ | $e_c$ | $e_f$ | $e_n$ | $R/10^{-1}$nm | $r_1/10^{-1}$nm | $r_2/10^{-1}$nm | $r_3/10^{-1}$nm | $n_1$ | $n_2$ | $n_3$ | $E_1$/(kJ·mol$^{-1}$) | $E_c$/(kJ·mol$^{-1}$) |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | 2.0929 | 0.4220 | 1.2600 | 3.7749 | 1.2251 | 0 | 1.3143 | 2.8582 | 3.3004 | 4.6675 | 0.4143 | 0.0759 | 0.0004 | 611.05 | 730.00 |
| 0.1 | 2.1643 | 0.4361 | 1.3029 | 3.9033 | 1.1967 | 0 | 1.3087 | 2.8395 | 3.2788 | 4.6369 | 0.4277 | 0.0795 | 0.0004 | 612.32 | 729.53 |
| 0.2 | 2.2337 | 0.4495 | 1.3445 | 4.0277 | 1.1723 | 0 | 1.3036 | 2.8221 | 3.2587 | 4.6085 | 0.4406 | 0.0828 | 0.0005 | 611.94 | 727.30 |
| 0.3 | 2.3006 | 0.4628 | 1.3848 | 4.1482 | 1.1518 | 0 | 1.2990 | 2.8060 | 3.2401 | 4.5822 | 0.4532 | 0.0861 | 0.0005 | 610.00 | 723.41 |
| 0.4 | 2.3652 | 0.4757 | 1.4238 | 4.2647 | 1.1353 | 0 | 1.2949 | 2.7911 | 3.2229 | 4.5579 | 0.4653 | 0.0892 | 0.0005 | 606.58 | 717.96 |
| 0.5 | 2.4274 | 0.4883 | 1.4613 | 4.3770 | 1.1230 | 0 | 1.2914 | 2.7774 | 3.2071 | 4.5355 | 0.4771 | 0.0922 | 0.0006 | 601.77 | 711.05 |
| 0.6 | 2.4874 | 0.5004 | 1.4973 | 4.4852 | 1.1148 | 0 | 1.2882 | 2.7649 | 3.1927 | 4.5151 | 0.4884 | 0.0950 | 0.0006 | 595.65 | 702.77 |
| 0.7 | 2.5451 | 0.5121 | 1.5319 | 4.5891 | 1.1109 | 0 | 1.2856 | 2.7535 | 3.1795 | 4.4965 | 0.4994 | 0.0978 | 0.0006 | 588.32 | 693.23 |
| 0.8 | 2.6005 | 0.5233 | 1.5651 | 4.6889 | 1.1111 | 0 | 1.2833 | 2.7432 | 3.1676 | 4.4797 | 0.5099 | 0.1003 | 0.0007 | 579.85 | 682.52 |
| 0.9 | 2.6537 | 0.5340 | 1.5970 | 4.7846 | 1.1154 | 0 | 1.2815 | 2.7340 | 3.1569 | 4.4646 | 0.5200 | 0.1027 | 0.0007 | 570.35 | 670.75 |
| 1 | 2.7045 | 0.5440 | 1.6280 | 4.8765 | 1.1235 | 0 | 1.2801 | 2.7257 | 3.1474 | 4.4511 | 0.5297 | 0.1050 | 0.0007 | 559.92 | 658.00 |

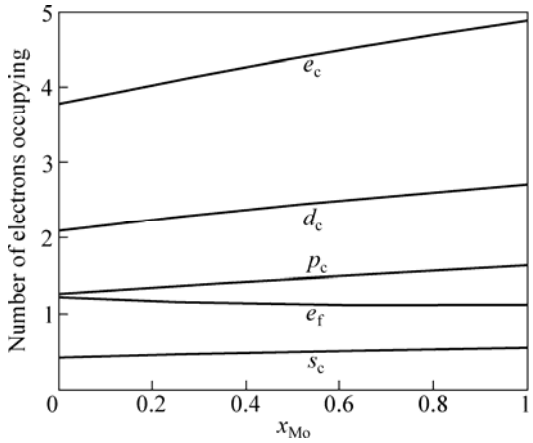


**Fig. 1** Electronic structure of disordered $Nb_{(1-x)}Mo_x$ alloys system as function of composition $x_{Mo}$

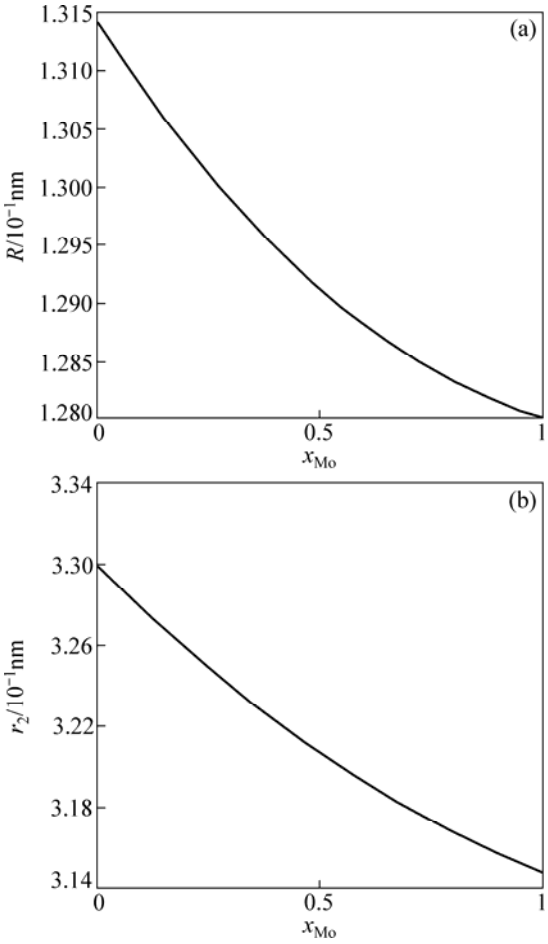


**Fig. 2** Single bond radius (a) and lattice constants (b) of disordered $Nb_{(1-x)}Mo_x$ alloys system as function of composition $x_{Mo}$

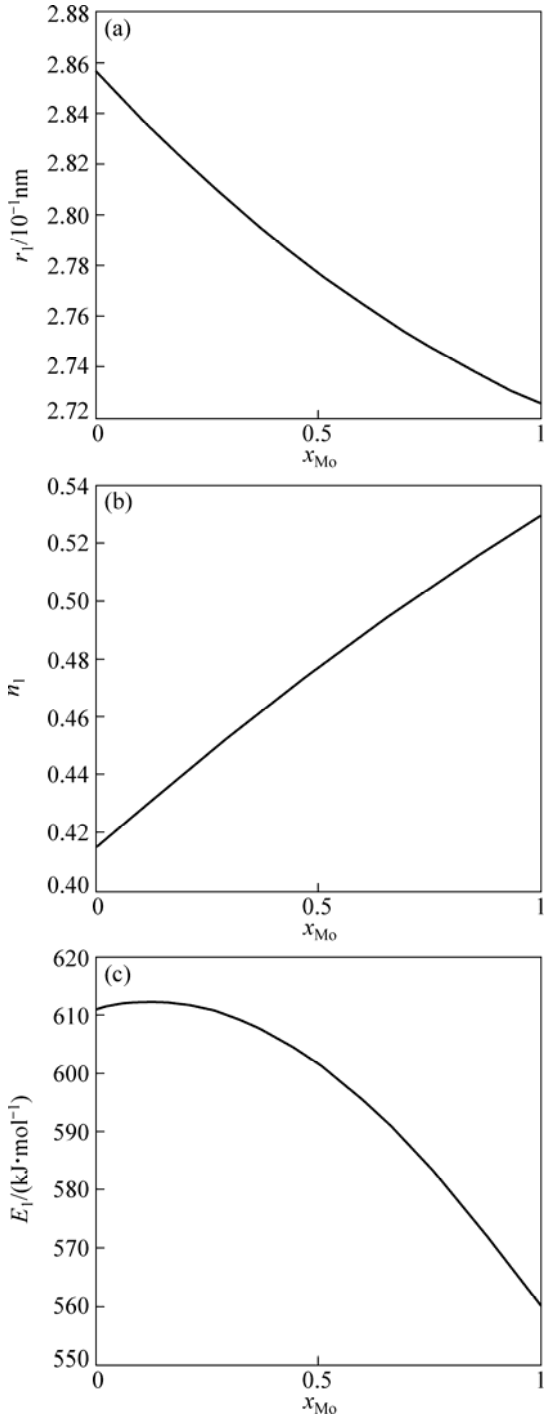


**Fig. 3** The nearest neighbor bond length (a), number of electrons (b) and bond energies (c) of disordered $Nb_{(1-x)}Mo_x$ alloys system as function of composition $x_{Mo}$

# 5 Conclusions

1) On the basis of idea of systematic science of alloys and experimental lattice constants and heats of formation, comprehensively considering the energy, volume and electronic structure of alloys, the ninth equation was determined as the interaction equation of Nb−Mo alloys system.

2) The structural parameters and properties of Nb and Mo characteristic atoms sequences and corresponding characteristic crystals sequences were determined in Nb−Mo alloys system. The electronic structures and physical properties of disordered

$Nb_{(1-x)}Mo_x$ alloys system were calculated according to concentration of characteristic atoms of disordered alloys and basic information of characteristic atom sequences and characteristic crystal sequences.

3) The change trend of physical properties is the same as that of electronic structure.

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# BCC 结构 Nb−Mo 合金系的特征原子序列及无序合金的性质


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**摘 要**：根据系统合金科学的思想，结合实验晶格常数和生成热，综合考虑合金能量、体积、原子状态之间的相互关系，确定 BCC 结构 Nb−Mo 合金系的相互作用方程为第 9 方程；同时，确定 Nb−Mo 合金系中 Nb 和 Mo 特征原子序列和特征晶体序列的基本信息；根据无序合金的特征原子浓度计算了无序 $Nb_{(1-x)}Mo_x$ 合金的电子结构和物理性质，其物理性质的变化趋势与电子结构的变化极其一致。



**关键词**：Nb−Mo 合金系；特征原子序列；无序合金；性质

**(Edited by YANG Hua)**