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Ab initio study of chemical effect on structural properties of Ti–Al melts

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We study chemical effect on the structural properties of Ti–Al melts, with the Al concentration systematically changed, via *ab initio* molecular dynamics simulations. By calculating the partial coordination numbers, we find a preferred connection between the nearest neighbors for Al–Ti pairs. This induces an excess Ti coordination in the cluster characterized by local five-fold symmetry in Voronoi tessellation. Structural entropy measured from the diversity of Voronoi polyhedrons shows an intriguing non-monotonic tendency with concentration: it first decreases to a minimum value at $Ti_{40}Al_{60}$, and then increases beyond this concentration. This implies a more ordered local structure induced by the chemical interaction at the intermediate compositions. The spatial correlation among the crystalline-like or the icosahedral-like clusters also exhibits the highest intensity for Al–Ti pairs, verifying the important role played by the chemical interaction in the local structure connectivity.

Keywords: Ti–Al alloys, chemical effect, atomic structure, *ab initio* simulations

PACS: 61.20.Ja, 61.25.Mv **DOI:** 10.1088/1674-1056/acd2c0

1. Introduction

TiAl alloys attract much attention in the application of engineering, e.g., in aerospace and automotive fields, owing to the lightweight and excellent mechanical properties.[1,2] When quenching the metallic melts at a fast-enough rate, crystallization can be avoided and the amorphous state of TiAl alloys is obtained. TiAl metallic glass (MG) has many unique properties that are preponderant to the crystalline counterparts, especially in mechanical performance and corrosion resistance.[3–5] Structural and dynamic properties of MGs can inherit from those of the liquid state, among which the most significant findings are the liquid-like regions and the associated string-like relaxation process.[6,7] From the aspect of inherency, liquid structure can significantly influence that of the metallic glass.

Investigating the structure of TiAl melts is enlightening in unveiling the structural feature for glass-forming ability or undercooling capability. Icosahedral short-range order (ISRO) is a peculiar local packing structure that is of five-fold symmetry but energetically stable. It was proposed first by Frank to explain the undercooling behaviors of liquids.[8] Existence of the ISRO was verified in diffraction experiment on pure Ti melts,[9,10] and liquid mixtures with Ti.[11,12] And soon after, it was found to be prevailing in metallic glass compounded with Zr and/or Cu.[13] They can even aggregate together to form some backbones or mediate-range order in the glass, thus stabilizing the supercooled liquids, and benefiting the glass-forming capability.[14,15]

Emergence of ISRO has also been reported in Ti–Al alloys. Upon cooling down, the population of ISRO grows up, and they can connect with each other by volume sharing to form icosahedral medium-range order.[16,17] In $TiAl_3$ metallic glass it has been found that the connecting mode of icosahedra, i.e., the face sharing and vertex sharing, can induce the split of the second peak in pair distribution function.[18] Additionally, the cooling rate is another important factor affecting the connections between icosahedral cluster and its defective structure.[19] However, all these researches are within the frame of classical molecular dynamics (MD) simulations. Reliability of the results from the classical MD simulations strongly depends on the accuracy of the empirical potential utilized.[20–23] An *ab inito* study on the structure of Ti–Al melts is desired to elucidate the detailed atomic structure including the ISRO.

Additionally, the alloy with Al element usually displays the feature of chemical interaction, due to the strong affiliation of Al with transition metals.[20,24,25] Structure change influenced by this interaction can be summarized as chemical short-range order (CSRO). For instance, the atomic radius of Al can be changed with composition in Au–Al melt[20] and shortened in Zr–Cu–Al MGs.[26] The affiliating propensity can trigger off the formation of chemically biased clusters in Zr–Ni–Al melts.[21] Inevitably, this chemical interaction can impose nontrivial influence on the formation of icosahedral clusters that is a short-range order (SRO) in topology. However, the interplay between the icosahedral packing and chemical interaction in Ti–Al melts has remained unclear in Ti–Al melts hitherto.

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2. Simulation details

To address the aforementioned questions, we conducted *ab initio* molecular dynamics (AIMD) simulations on Ti–Al alloys, with the Al concentration systematically changed, i.e., in $Ti_{100-x}Al_x$ alloys with $x = 0$, 20, 40, 60, 80, 100. The simulations were performed by using the Vienna *ab initio* simulation package (VASP),[27] with the electron–ion interaction described by the projected augmented-wave through using the generalized gradient approximation (GGA)[28] for the exchange–correlation function in the Perdew–Burke–Ernzerhof parameterization.[29] Plane-wave basis was used with an energy cutoff of 270 eV. Only the Γ points were used to sample the Brillouin zone. Newton's equations of motion were integrated in the velocity form by using the Verlet's algorithm in NVT canonical ensembles in time steps of 3.0 fs. The temperature was controlled by a Nosé thermostat.

A cubic simulation box containing 250 atoms was simulated with periodic boundary conditions applied to all the dimensions. The initial configuration was constructed at 2000 K with all atoms randomly placed in the cubic box. After a short-time relaxation (about 36 ps) the liquid samples were subsequently cooled down to 1500 K. Atom information is collected at this temperature to investigate the structural evolution with concentration. Cell size was adjusted according to the density measured in experiment.[30] At this density, the resulting pressure of the system does not exceed ± 4 kbar (1 bar $= 10^5$ Pa). For each alloy, the total relaxation time exceeds 60 ps, with the configurations in the first 12 ps discarded and the left ones used for data analysis.

3. Results and discussion

The microscopic structure of amorphous system can be described by the partial pair distribution function (PDF), $g_{\alpha\beta}(r)$, which gives the probability of finding an atom of type β at a distance r from the central atom of type α. The total PDF can be calculated by the partial ones via $g(r) = \sum_{\alpha\beta} c_\alpha c_\beta g_{\alpha\beta}(r)$.

Figure 1 shows the calculated total and partial PDFs in Ti–Al melts with various compositions. The shapes and positions of the first peaks are nearly unchanged with the Al concentration x_{Al} increasing. The first peak position is usually considered to be the diameter of the atom $R^{(1)}$. $R^{(1)}$ is found to be around 2.80 Å, 2.76 Å, 2.81 Å, 2.84 Å for total, Al–Al, Al–Ti, and Ti–Ti pairs, respectively [see Figs. 1(a)–1(d)]. The atomic diameters from Al–Al and Ti–Ti pairs are consistent with the values from Pauling radius,[31] where $R_{Al} = 1.429$ Å and $R_{Ti} = 1.467$ Å. This gives the atomic size ratio about 0.97, indicating a small size discrepancy between these two species.

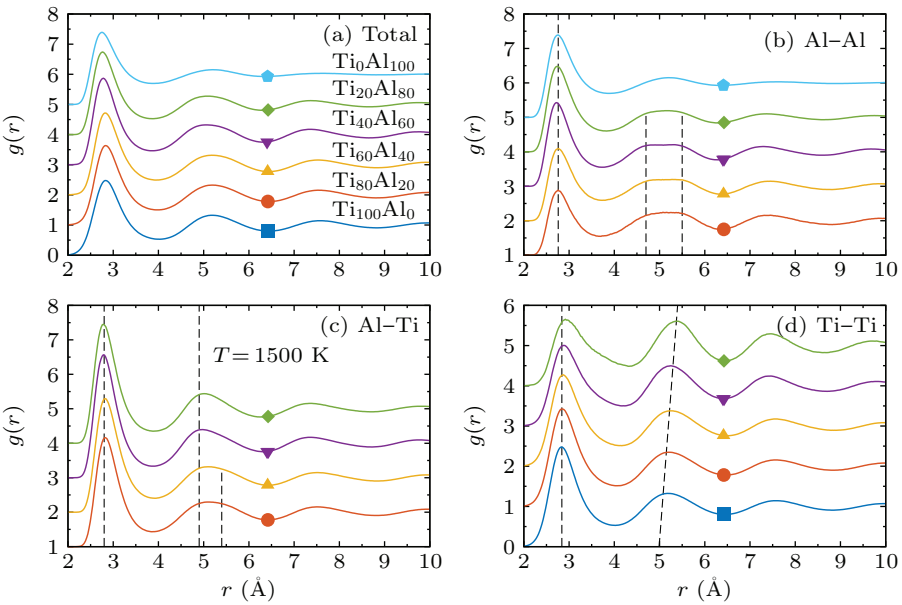


Fig. 1. Distance r-dependent pair correlation functions, $g(r)$, for various compositions in $Ti_{100-x}Al_x$ melts for (a) total, (b) Al–Al, (c) Al–Ti, and (d) Ti–Ti pairs, with vertical dashed lines marking the first peak position in panels (a)–(d) and the second peak position in panels (b)–(d).

Unlike the first peak, a tendency for the splitting of the secondary peak emerges in Al–Al pairs at around $r \approx 5$ Å [see the vertical dashed lines in Fig. 1(b)]. Position of the outer secondary peak is at about 5.5 Å. If the first peak position of total PDF is taken as the average atom diameter, i.e., $\overline{R^{(1)}} = 2.8$ Å, the outer secondary peak is at about 1.96 $\overline{R^{(1)}}$, almost twice the atomic diameter. This is a loose packing in the second nearest neighbor, consistent with the connection of two polyhedral clusters connected by vertices.[32] The inner secondary peak is located at around 4.7 Å, i.e., 1.67 $\overline{R^{(1)}}$, indicating a more efficient packing structure. If two tetrahedra are connected by sharing a face, which results in a tetragonal bipyramid, then the distance between their two vertices is $2\sqrt{6}/3 \approx 1.63$, close to the inner secondary peak. A similar

situation has been reported in Al–Au melts,[20] where the inner splitting secondary peak is located at about 1.68 $\overline{R^{(1)}}$ for Al–Au pairs. Similarly, the splitting tendency also emerges in Al–Ti pairs at $x_{\mathrm{Al}} = 20$ Å and 40 Å as shown in Fig. 1(c). In $Ti_{80}Al_{20}$ liquid and $Ti_{60}Al_{40}$ liquid, the inner and outer secondary peak are located at about $r = 4.9$ Å and 5.4 Å, respectively, coinciding with those of the Al–Al pairs. However, the splitting tendency gradually disappears with further increase of Al content, specifically, the splitting tendency is terminated at $x_{\mathrm{Al}} > 40$. This may be due to the increased population of the face-sharing clusters, since the valley in the splitting corresponds to this connection.[18,32] In contrast, the secondary peak position for Ti–Ti pairs monotonically shifts to larger distance with Al content increasing as seen in Fig. 1(d). The variations of the secondary peak of $g_{\mathrm{TiTi}}(r)$ and $g_{\mathrm{AlTi}}(r)$ with composition highlight that the connection of Ti–Ti pair and Al–Ti pair in the second neighbor shells are sensitive to chemical environment.

To quantify the chemical effect, we evaluate the chemical environment in the nearest neighbor shells with the partial coordination number, $Z_{\alpha\beta}$, which is the average neighbor number of neighbors of type β around the central atom of type α. It can be calculated by the partial PDF as follows:

$$Z_{\alpha\beta} = 4\pi\rho c_\beta \int_0^{r_c} r^2 g_{\alpha\beta}(r)\,\mathrm{d}r, \tag{1}$$

where ρ is the average number density, c_β is the concentration of atomic type β, and r_c is the first minimum distance in the corresponding partial PDF. The total coordination number for atom type α is $Z_\alpha = \sum_\beta Z_{\alpha\beta}$. In the case of random substitution, the neighbors around some atoms are randomly selected according to the concentration of species. This gives the ratio of coordination numbers in random substitution: $Z_{\alpha\beta}/Z_\beta = c_\alpha$, independent of the type of the central atom.

The calculated ratios of the coordination numbers are shown in Fig. 2. The dashed lines are the expectation from random substitution. Clear deviation of the concentration is observed around central Al atoms as seen in Fig. 2(a). The coordinating Ti atoms around Al atoms are found to be more than those expected from the random substitution, but the surrounding Al atoms are less than expected. This indicates that Al atoms prefer to connect with Ti atoms but avoid connecting with themselves. The excess value to the random substitution reaches a maximum value at $x_{\mathrm{Al}} = 40$. The preferred connection for Ti–Al nearest neighbors and the avoidance for Al–Al ones indicate a strong affiliation between Al and Ti atoms. The affiliation tendency difference should be induced by the chemical interaction, analogous to the reported phenomenon of the concentration-biased clusters in the nearest neighbor shells in Zr–Ni–Al melt.[21] In contrast, the coordinating concentration almost coincides with that of the random substitution around the central Ti atoms [see Fig. 2(b)]. This implies that the biased concentration is mainly caused by the chemical interaction with Al atoms. Significantly high negative values of experimental data are found for the excess molar volume, which may relate to the concentration-biased connection in Al–Ti melts.[30]

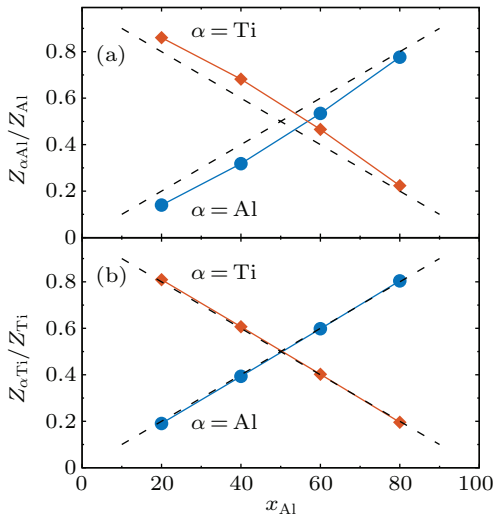


Fig. 2. Ratio of coordinating numbers around central (a) Al atoms and (b) Ti atoms as a function of x_{Al}, with dashed lines representing the expected value from random substitution.

It is interesting to see how the geometric packing of local structures, e.g., the packing of icosahedral clusters (ISRO), can be affected by the occurrence of the chemically preferred short-range order. To this end, we utilize the Voronoi tessellation method to characterize the local structure in the melt. The Voronoi index $\langle n_3, n_4, n_5, n_6\rangle$, where n_i denotes the number of i-edged faces of the polyhedral cluster surrounding an atom, is used to characterize the packing of the nearest neighbor atoms around a central atom.[33] Based on the Voronoi analysis, the local five-fold symmetry (LFFS) is defined as the fraction of the pentagon faces in the polyhedron: $d_5 = n_5/\sum_i n_i$.[34] The LFFS has been found to be a good indicator for the mechanical property of metallic glasses.[35] Typically, d_5 is close to 1 for clusters of icosahedral-like order, and it is close to zero for clusters of crystalline-like order (for which triple or quadruple symmetry dominates).

Distribution probability of d_5 is Gaussian-like in the liquid [see Fig. 3(a)]. The population of perfect icosahedral clusters ($d_5 = 1$) is small, and the highest percentage is only about 1.8% in $Ti_{40}Al_{60}$ melt. This indicates that the most of icosahedral clusters are distorted in liquid. Interestingly, the population of icosahedral-like clusters ($d_5 > 0.5$) is higher in the mixture than that in pure metal, while the population of crystalline-like clusters ($d_5 < 0.5$) is smaller in the mixture. This gives a non-monotonic evolution of the population of the icosahedral-like clusters with Al concentration. As the atomic size ratio is small ($= 0.97$), we conclude that the evolution of atomic packing structure can be dominated by the chemical

interaction, rather than the entropic effect from the mixing of two different hard spheres.

The preferred connection for Al–Ti pairs can affect the constituents of the local structures. For this we calculate the concentration of the coordinating atoms in the nearest neighbor shell. In the case of random mixing, the calculated probability (e.g. $f_{\mathrm{Ti}}^{\mathrm{shell}}$ for Ti atoms) should be equal to that of its composition (e.g. x_{Ti} for Ti atoms). However, it is found that the $f_{\mathrm{Ti}}^{\mathrm{shell}}$ is larger than x_{Ti} in all the compositions for most of the local clusters classified by LFFS [Fig. 3(b)]. The only exception is that $f_{\mathrm{Ti}}^{\mathrm{shell}}$ is smaller than x_{Ti} for the crystalline-like structure ($d_5 < 0.5$) in $Ti_{20}Al_{80}$ melt. Nevertheless, the excess Ti concentration in the nearest neighbor indicates the formation of CSRO, especially in the icosahedral-like structure. This coincides with the finding of the preferred connection between Ti and Al atoms.

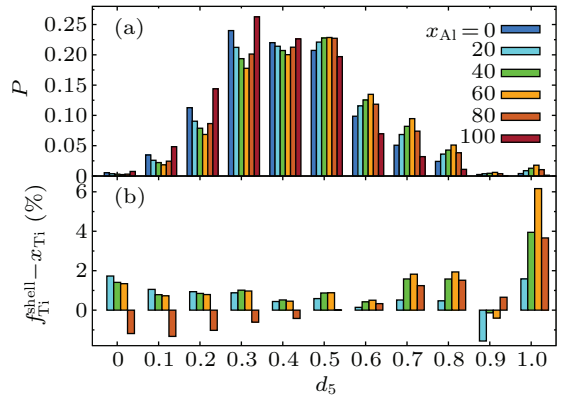


Fig. 3. (a) Distribution probabilities of local five-fold symmetry (LFFS) d_5; (b) Ti concentrations in the nearest neighbor shells of polyhedral d_5, $f_{\mathrm{Ti}}^{\mathrm{shell}}$, subtracted by the concentration of Ti (x_{Ti}) in the alloy.

Although the LFFS clusters can exhibit the evolution tendency of the population with concentration, an overall ordered or disordered extent in liquid is still unclear. For this, we use the structural entropy or Shannon entropy to measure the local structure diversity in the liquid:[36]

$$S = -\sum_{i=1}^{N} P_i \log P_i. \tag{2}$$

Here, P_i is the percentage of Voronoi polyhedron of type i in the liquid. For the ordered system with only one type of local structure, $S = 0$. For the disordered system where the probabilities of all the local structures are the same, S reaches its maximum value.

Figure 4(a) shows the composition evolution of the calculated structural entropy in Al–Ti system. Interestingly, a non-monotonic evolution is observed: the structural entropy first decreases then increases, with a minimum emerging at $x_{\mathrm{Al}} = 60$. Thus, the liquid structure is more ordered in the middle composition. As alluded above, this relatively ordered structure can be due to the chemical interaction emerging in the middle compositions. In experiment and AIMD simulation, it is found that the mixing enthalpy also shows a non-monotonic evolution; it first decreases, then increases, with a minimum value reported at $x_{\mathrm{Al}} \approx 60$,[37,38] coinciding well with the composition of the minimum local structural entropy found here. The most negative mixing enthalpy verifies the strongest chemical interaction at this composition, and can lead to the most ordered local structure.

The chemical interaction may also affect the spatial correlation of local structures. To this end, we calculate the spatial correlation index C_{ij} between two polyhedral clusters of type i and j, which is represented by LLFS (d_5) and defined as $C_{ij} = p_{ij}/p_{ij}^0 - 1$, where p_{ij} is the probability of LFFS of types i and j being the nearest neighbors in the simulated alloys, and p_{ij}^0 is the probability of these two clusters in random mixing.[15] Therefore, a positive value of C_{ij} indicates the preferred correlation between clusters i and j, while a negative value represents the anticorrelation (i.e., the atoms of these two types avoid being nearest neighbors).

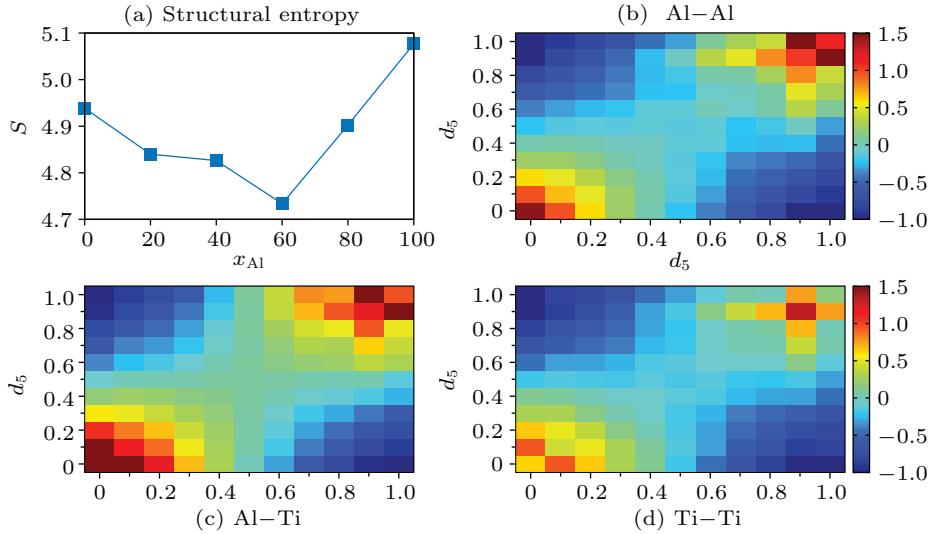


Fig. 4. (a) Voronoi structural entropy as a function of composition; patial correlation of different LFFS clusters for the nearest (b) Al–Al pairs, (c) Al–Ti pairs, and (d) Ti–Ti pairs in $Ti_{40}Al_{60}$.

To distinguish the correlation between different atomic pairs, we calculate the pair-type dependent C_{ij}, with the results shown in Figs. 4(b)–4(d) for Al–Al, Al–Ti, and Ti–Ti pairs, respectively. The correlation index is positive in the diagonal direction (from bottom left to top right), which represents the correlation between alike clusters. The largest values appear in the bottom left corner and the top right corner, indicating that the correlation among the icosahedral-like clusters or the crystalline-like clusters is the strongest. Of the different atomic pairs, the Al–Ti pair has the largest maximum correlation extent, Al–Al pair has the intermediate one, and the Ti–Ti pair has the smallest one. This, exactly, corresponds to the chemical interaction found in Fig. 2. Although the results shown in Fig. 4 are from $Ti_{40}Al_{60}$ melt, we find that this conclusion remains unchanged with the mixing concentration changing. This shows that the chemical interaction plays an important role in determining the connection of local structures in Ti–Al alloys.

4. Conclusions

Ab initio molecular dynamics simulations are conducted to study the chemical effect on the structural properties in Ti–Al alloys, for which the Al concentration is systematically changed. The liquid structure is measured by pair correlation functions, which shows a splitting tendency in the secondary peaks in the intermediate compositions in Al–Al and Al–Ti pairs. The chemical effect is characterized by the partial coordination numbers, finding that there exists a preferred connection for Al–Ti nearest pairs. This effect is also exhibited as the excess Ti coordinating atoms in the polyhedral clusters: those atoms are characterized by the local five-fold symmetry parameter. With Al concentration increasing, the structural entropy shows a non-monotonic behavior: it first decreases to a minimum value at $Ti_{40}Al_{60}$, then increases beyond this point. This indicates the relatively ordered local structure induced by chemical interaction. The spatial correlation displays the strongest intensity in the crystalline-like or the icosahedral-like clusters for Al–Ti pairs, coinciding with the preferred connection found in these pairs.

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References

[1] Appel F, Brossmann U, Christoph, Eggert S, Janschek P, Lorenz U, Mullauer J, Oehring M and Paul J D 2000 *Adv. Eng. Mater.* **2** 699
[2] Aguilar J, Schievenbusch A and Kattlitz O 2011 *Intermetallics* **19** 757
[3] Wang W H, Dong C and Shek C H 2004 *Mater. Sci. Eng. R.* **44** 45
[4] Inoue A 2000 *Acta Mater.* **48** 279
[5] Zhang J Y, Zhou Z Q, Zhang Z B, Park M H, Yu Q, Li Z, Ma J, Wang A D, Huang H G, Song M, Guo B S, Wang Q and Yang Y 2022 *Mater. Futures* **1** 012001
[6] Chang C, Zhang H P, Zhao R, Li F C, Luo P, Li M Z and Bai H Y 2022 *Nat. Mater.* **21** 1240
[7] Wang Q, Shang Y H and Yang Y 2023 *Mater. Futures* **2** 017501
[8] Frank F C 1952 *Proc. R. Soc. Lond. Ser. A* **215** 43
[9] Schenk T, Holland-Moritz D, Simonet V, Bellissent R and Herlach D M 2002 *Phys. Rev. Lett.* **89** 075507
[10] Lee G W, Gangopadhyay A K, Kelton K F, Hyers R W, Rathz T J, Rogers J R and Robinson D S 2004 *Appl. Phys. Lett.* **93** 037802
[11] Kelton K F, Lee G, Gangopadhyay A K, Hyers R, Rathz T J and Rogers J R 2003 *Phys. Rev. Lett.* **90** 195504
[12] Lee G, Gangopadhyay A K, Hyers R W, Rathz T J, Rogers J R, Robinson D S, Goldman A I and Kelton K F 2008 *Phys. Rev. B* **77** 184102
[13] Cheng Y Q and Ma E 2011 *Prog. Mater. Sci.* **56** 379
[14] Peng H L, Li M Z, Wang W H, Wang C Z and Ho K M 2010 *Appl. Phys. Lett.* **96** 021901
[15] Li M, Wang C Z, Hao S G, Kramer M J and Ho K M 2009 *Phys. Rev. B* **80** 184201
[16] Xie Z C, Gao T H, Guo X T, Qin X M and Xie Q 2014 *Comput. Mater. Sci.* **95** 502
[17] Xie Z C, Gao T H, Guo X T, Qin X M and Xie Q 2014 *J. Non-Cryst. Solids* **394–395** 16
[18] Tahiri M, Hassani A, Sbiaai K and Hasnaoui A 2018 *Comput. Condensed Matter* **14** 74
[19] Liu Z, Li L, Gao T, Xie Q, Chen Q, Liang Y, Tian Z and Wang B 2021 *Phys. Status Solidi B* **258** 2100083
[20] Peng H L, Voigtmann T, Kolland G, Kobatake H and Brillo J 2015 *Phys. Rev. B* **92** 184201
[21] Peng H L, Yang F, Liu S T, Holland-Moritz D, Kordel T, Hansen T and Voigtmann T 2019 *Phys. Rev. B* **100** 104202
[22] Wen T, Zhang L, Wang H, Weinan E and Srolovitz D J 2022 *Mater. Futures* **1** 022601
[23] Zhai B and Wang H P 2023 *Comput. Mater. Sci.* **216** 111843
[24] Das S K, Horbach J, Koza M M, Mavila Chathoth S and Meyer A 2005 *Appl. Phys. Lett.* **86** 011918
[25] Yuan C C, Yang F, Kargl F, Holland-Moritz D, Simeoni G G and Meyer A 2015 *Phys. Rev. B* **91** 214203
[26] Cheng Y Q, Ma E and Sheng H W 2009 *Phys. Rev. Lett.* **102** 245501
[27] Kresse G and Hafner J 1993 *Phys. Rev. B* **47** 558
[28] Perdew J P, Burke K and Ernzerhof M 1996 *Phys. Rev. Lett.* **77** 3865
[29] Kresse G and Joubert J 1999 *Phys. Rev. B* **59** 1758
[30] Wessing J and Brillo J 2017 *Metall. Mater. Trans. A* **48** 868
[31] Pauling L 1947 *J. Am. Chem. Soc.* **69** 542
[32] Pan S P, Qin J Y, Wang W M and Gu T K 2011 *Phys. Rev. B* **84** 092201
[33] Liu Q and Guan P F 2018 *Acta Phys. Sin.* **67** 178101 (in Chinese)
[34] Li M Z, *et al.* 2017 *Chin. Phys. B* **26** 016104
[35] Peng H L, Li M Z and Wang W H 2011 *Phys. Rev. Lett.* **106** 135503
[36] Peng H L, Li M Z and Wang W H 2013 *Appl. Phys. Lett.* **102** 131908
[37] Xu T T, Li J Y, X R, Qin J Y, Ruan Y and Li H 2022 *J. Phase Equilib. Diffus.* **43** 585
[38] Witusiewicz V T, Bondar A A, Hecht U, Rex S and Velikanova T Y 2008 *J. Alloys Compd.* **465** 64