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# Vitrification and crystallization of metallic liquid under pressures

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## Abstract

Using molecular dynamics simulation with the embedded atom method, the structural properties of liquid NiAl in a pressure range of 0–20 GPa are investigated with a quenching rate of 2 K ps<sup>-1</sup>. Not only is vitrification of liquid at low temperature detected, but also crystallization by change of average atomic volume as a function of temperature. Convincing evidence is presented that the applied pressure strongly affects the vitrification and crystallization of metallic liquid. The simulated glass transition temperature  $T_g$  increases with pressure by 38.4 K GPa<sup>-1</sup> within the range 0–10 GPa, while external pressure induces crystallization of metallic liquid within the pressure range 10–20 GPa, and the crystallization temperature  $T_c$  increases with a slope of 6.4 K GPa<sup>-1</sup>. Therefore, the critical pressure for the formation of metallic glass at this cooling rate is estimated to be 10 GPa. The competition between the densification and the suppression of atomic diffusion in the liquid by pressure is able to explain the vitrification and crystallization behaviours of the liquid. Our present work provides a possible guidance for an experiment to study the pressure effect on the glass transition and crystallization process in metallic liquid.

(Some figures in this article are in colour only in the electronic version)

## 1. Introduction

For a long time much attention has been given to considering the effect of cooling rate on metallic glass formation since a metallic glass was first made by rapid quenching in 1960 [1]. The metallic liquid can undergo a glass transition if the cooling rate is fast enough to suppress the nucleation and growth of the crystalline phase [2, 3]. Pressure, similar to cooling rate, is also an important variable that affects the glass transition, being one of the key issues regarding the validity of existing various theories and establishing new theories [2, 4]. Most experimental results [4, 5] have been reported from studies of the formation of the Zr-based

bulk metallic glass (BMG) under high pressure by means of heating the metallic glass to the glass transition temperature, and they indicate that the glass transition temperature increases with pressure. Furthermore, high pressure suppresses the crystallization in the supercooled liquid [6], which favours the formation of metallic glass. Recently, the crystallization behaviour of metallic glass under pressure, for example Zr-based [7] and Cu-based [8] BMG, has been reported. This demonstrates that applied pressure can change the crystallization process and that the crystallization temperature is enhanced with increasing external pressure. Generally, the glass is viewed as a 'frozen liquid' [9]; thus the supercooled liquid phase zone from glassy to crystalline state might link to the relationship of that supercooled zone from the liquidus line to the crystalline state. The crystallization of metallic glass is to some extent similar to the crystallization of metallic liquid, both undergoing the transition from a disordered to ordered state, since the crystallization temperature of a metallic liquid increases with pressure. This seems to be incompatible. The pressure on a liquid metal has complex effects: on the one hand, an increase of pressure restricts the atomic diffusion of the liquid, which favours a glass transition since atomic diffusion over a long range is required for these crystallization processes. On the other hand, the increased pressure in a liquid causes a reduction of the free volume and an increase in the densification, which favours crystallization since the crystallization of a liquid requires volume contraction. The pressure plays a very important role in the competition of vitrification and crystallization during the cooling process. In this paper we want further to investigate what would happen on earth as an external pressure is applied to the liquid. Does it favour the formation of glass or crystal at the same cooling rate?

In recent years, there has been much progress in the understanding of the pressure effect on a metallic liquid. Some work focuses on the investigation of a discontinuous structural phase transition of metallic melts induced by high temperature and high pressure [10–13]. Pressure is responsible for the disappearance of the medium-range order in the form of the free volume in liquid Se [14]. Recently liquid Ge has been investigated in a wide pressure and temperature range (namely 0–16 GPa, 298–498 K) by extended x-ray absorption fine structure spectra [15]. So far, experimental studies on the influence of pressure on a metallic liquid are not adequate and most of them have been limited to lower pressures, although Shen investigated the structure of liquid iron at pressures up to 58 GPa, measured by x-ray scattering in a laser heated diamond anvil cell [16]. This imbalance is apparently not due to the lack of scientific importance of the studies, but to the experimental difficulties arising from the extreme conditions required to obtain metallic liquid. Furthermore, experiments have not allowed us to measure directly the influence of pressure on atom movement to a particular neighbour in a solid or the reorganization of local structure. Therefore, how pressure affects a liquid-to-solid transition is hardly possible to be determined by experiment. Computer simulations provide an opportunity to study these processes at an atomic level. Recently, molecular dynamics has been used to simulate the local structure of liquid germanium under pressure [17]. Li has compared the local order of liquid Al at normal pressure with that at a pressure of 9 GPa by molecular dynamics simulation [18]. The main purpose of the present work is to explore the effect of different pressures on the cooling process of liquid metal. The interaction potential of atoms is the basis for the molecular dynamics simulation. The Ni–Al interaction developed by Chen and Voter proved to be accurate to describe the liquid structure and glass formation of NiAl in our earlier work [19]. The simulated melting temperature is 1850 K, close to its melting point of 1913 K, which makes it a good candidate in our simulation.

This paper is organized as follows. In section 2 we report the details of the simulation process. Section 3 presents the structural parameters used to describe the phase transition from liquid to solid under various pressures. Section 4 presents the results and discussion and finally we conclude in section 5.

**Table 1.** The model parameters in the Chen and Voter EAM many-body potential.

Element	$D_M$ (eV)	$R_M$ (Å)	$\alpha_M$ (Å <sup>-1</sup> )	$\beta$ (Å <sup>-1</sup> )	$a_0$ (Å)	$E_{\text{coh}}$ (eV)
Al	3.7760	2.1176	1.4859	3.3232	—	—
Ni	1.5335	2.2053	1.7728	3.6408	—	—
Al–Ni	3.0322	2.0896	1.6277	—	2.88	4.51

## 2. MD simulation process

The interactions between all atoms are calculated using the embedded atom method (EAM), developed by Chen and Voter [20], having the following form:

$$E_{\text{tot}} = \sum_i F_i(\bar{\rho}_i) + \frac{1}{2} \sum_{i,j} \Phi_{ij}(r_{ij}). \quad (1)$$

Here  $\Phi_{ij}$  is the pair-interaction energy between atoms  $i$  and  $j$  at positions  $\vec{r}_i$  and  $\vec{r}_j$ , and  $F_i$  is the embedding energy of atom  $i$ . The  $\bar{\rho}_i$  in equation (1) is the host electron density at site  $i$  induced by all other atoms in the system, and it can be given by

$$\bar{\rho}_i = \sum_{j \neq i} \rho_j(r_{ij}). \quad (2)$$

$F_i(\bar{\rho}_i)$  provides the volume-dependent, many-body contribution to the energy. The pair interaction and density function are given as follows:

$$\Phi(r) = D_M \{1 - \exp[-\alpha_M(r - R_M)]\}^2 - D_M \quad (3)$$

$$\rho(r) = r^6 [e^{\beta r} + 2^9 e^{-2\beta r}]. \quad (4)$$

Here  $D_M$ ,  $\alpha_M$ ,  $R_M$ , and  $\beta$  are model parameter, and we define  $F_i(\bar{\rho}_i)$  by requiring that the energy of the fcc crystal is given by

$$E_{\text{fcc}}(a^*) = -E_{\text{coh}}(1 + a^*)e^{-a^*}. \quad (5)$$

Here  $E_{\text{coh}}$  is the fcc cohesive energy and  $a^*$  is a reduced lattice constant defined by

$$a^* = (a/a_0 - 1)/(E_{\text{coh}}/9B\Omega)^{1/2}. \quad (6)$$

Here  $a$  is the lattice constant,  $a_0$  is the equilibrium lattice constant,  $B$  is the bulk modulus, and  $\Omega$  is the equilibrium atomic volume. Thus, knowing  $E_{\text{coh}}$ ,  $a_0$ , and  $B$ , the embedding function is defined by requiring that the crystal energy from equation (5) matches the energy from equation (1) for all values of  $a^*$ . The model parameters are listed in table 1, and detailed information can be found in [20].

Now we list the details of the simulation conditions applied in this work. Molecular dynamics in the usual classical form was performed with a binary alloy system containing 512 Ni atoms and 512 Al atoms in a cubic box under three-dimensional periodic boundary conditions. The initial configuration for the preliminary simulation is constructed to B2 structure solid. Newton's equations of motion are solved by a Verlet algorithm [21] with a time step of 1 fs. The damped force method [22] is used to decrease the temperature by forcing the bath temperature to change linearly at each time interval. The system is first equilibrated at 600 K under a constant temperature and constant pressure condition and the liquid structure is realized by sequentially increasing the temperature of the system at the heating rate of 4 K ps<sup>-1</sup>. The system is judged to have melted by studying the relation between the average atomic volume and temperature. After running 10 000 time steps to equilibrate the structure in the liquid phase at 2200 K under various pressures (0–20 GPa), the system is cooled at the same cooling rate from 2200 to 400 K. At given temperatures, another simulation with 1000 time steps is performed for the structural and thermodynamic average.

### 3. The structural analysis technique

Specifically, the pair correlation function (PCF) as well as the pair analysis (PA) technology is analysed in detail to explore the structural transition under different pressures during the cooling process.

#### 3.1. Pair correlation function (PCF)

The PCF can be obtained by Fourier transformation of the x-ray diffraction factor  $S(Q)$ . The probability  $g(r)$  has been widely used to describe the structure characterization of liquid and amorphous states. It is defined as

$$g_{ij}(r) = \frac{L^3}{N_i N_j} \left\langle \sum_{\alpha=1}^{N_i} n_{\alpha j}(r) / (4\pi r^2 \Delta r) \right\rangle. \quad (7)$$

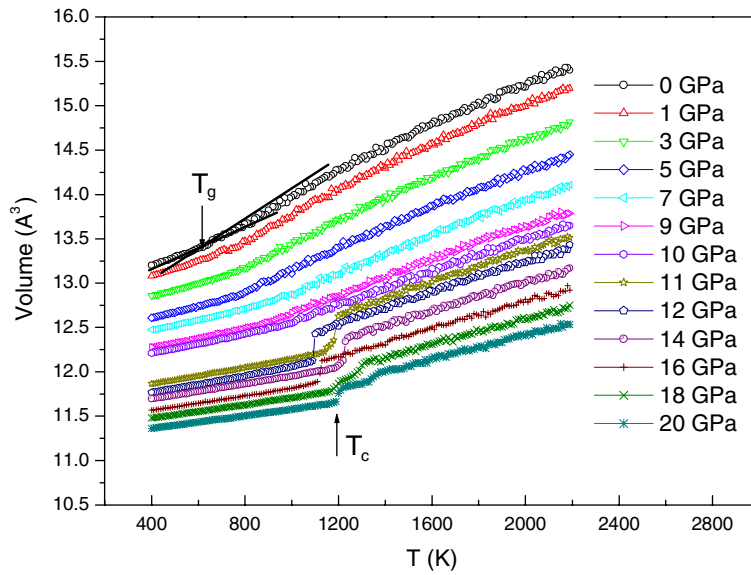
Here  $g_{ij}(r)$  is the probability of finding an atom in the range from  $r$  to  $r + \Delta r$ , and  $L$  is the cell length of the box in the simulation.  $N_i$  and  $N_j$  are the numbers of atoms  $i$  and  $j$  respectively in the system, and  $n_{\alpha j}$  is the averaged number of  $j$ -type atoms around  $i$ -type atoms in the sphere shell ranging from  $r$  to  $r + \Delta r$ , where  $\Delta r$  is the calculation step.

#### 3.2. Pair analysis (PA) technique [23]

To characterize the structural transition of a liquid under various pressures, we adopt a common technique used by Honeycutt and Anderson [23]. Four variables ( $i, j, l, m$ ) are used to distinguish bonded pairs in the PA technique. If any atom system A–B forms a bond,  $i = 1$ ; otherwise  $i = 2$ . Here a bond means that the pair of atoms is closer than a given cutoff distance, chosen to equal the position of the first minimum in the appropriate pair correlation function. The variable  $j$  denotes the number of near neighbours which form bonds with both atom A and atom B. The variable  $l$  represents the number formed among near neighbours which form bonds with both atom A and atom B. The variable  $m$  represents the way of linking of bonds with both atom A and atom B. If these bonds link in turn,  $m = 1$ ; otherwise  $m = 2$ . Based on the PA formula, different kinds of bonds can be obtained by computer. For example, the 1551 bonded pairs represent the two root pair atoms with five common neighbours that have five bonded pairs which form a pentagon of near-neighbour contacts. A similar analysis holds for other bonded pairs. It is necessary to point out the 1421 bonded pair is the characteristic pairs of fcc crystal; the 1421 and 1422 bonded pairs are related to the hcp crystal; there are many 1661 and 1441 bonded pairs in bcc crystal.

### 4. Results and analysis

Many metallic liquids are not glass formers from an experimental point of view, because the critical cooling rate for glass formation is always too high to be easily accessible in experiments. But molecular dynamics simulation can provide important insights by allowing one to determine quantities that are difficult to access in real experiments, for example high pressure. Figure 1 presents the temperature dependence of average atomic volume under various pressures, quenching from 2200 to 400 K with a cooling rate of 2 K ps<sup>-1</sup>. The decrease in volume is seen as the external pressure is applied to the liquid. Only a subtle change of slope in the volume versus temperature is observed with a pressure less than 10 GPa; we attribute the change of slope to solidification into an amorphous state. Up to 10 GPa, the glassy state is retained without a clear indication of crystallization at the simulated cooling rate. The patterns

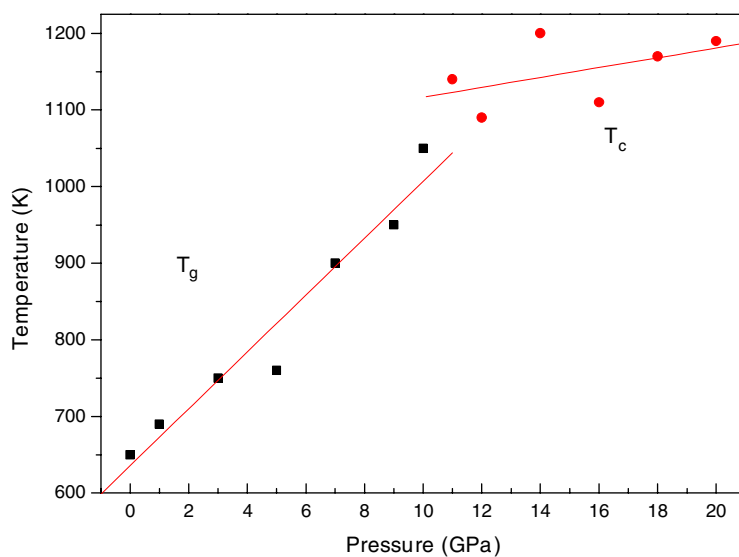


**Figure 1.** Average atomic volume of NiAl alloy as a function of temperature with the same cooling rate of  $2 \text{ K ps}^{-1}$ . This shows that the glass transition temperature increases with increasing pressure up to 10 GPa. When the pressure applied to the liquid is higher than 10 GPa, the crystalline phase forms at a lower temperature.

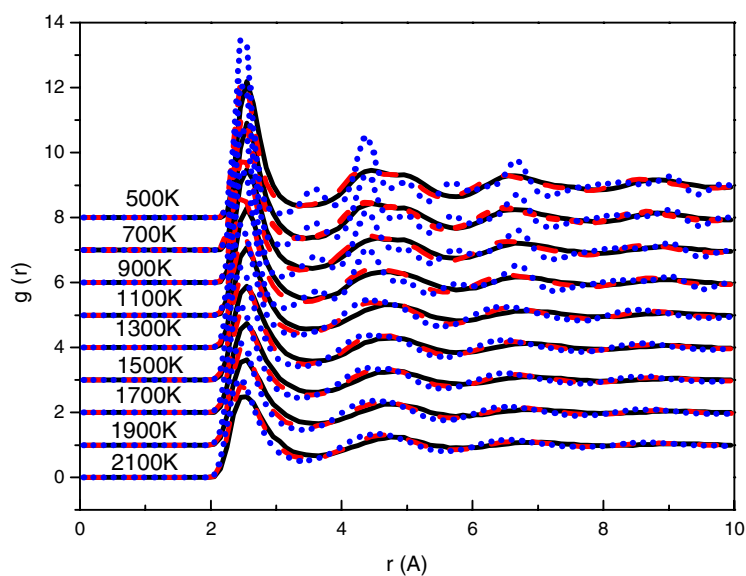
are recorded every 10 K to determine the glass formation temperature  $T_g$ .  $T_g$  for a model system is defined by the temperature at the intersection of the extrapolations of the liquid and glassy plots. It is estimated to be 600 K at 0 GPa and 1050 K at 10 GPa. In figure 2, we present the average increase of the glass transition temperature with a pressure of  $38.4 \text{ K GPa}^{-1}$ , much higher than that of the bulk metallic glasses with a pressure of  $4.4 \text{ K GPa}^{-1}$  [4] and  $5.6 \text{ K GPa}^{-1}$  [5] for Zr-based BMG. The discrepancies may be due to the fact that high cooling rate induces a higher glass forming ability since the simulation is under a controlled dynamics process. This result indicates that  $T_g$  is sensitive to the pressure, and that high pressure could be used to evaluate the glass forming ability of the melts. High pressure suppresses the crystallization in the supercooled liquid through increasing its viscosity, which favours the formation of glass at a higher temperature [6].

When the pressure applied is higher than 10 GPa, the glass formation temperature no longer increases with pressure. Interestingly, a rapid decrease in volume in the temperature region between 1100 and 1200 K, presented in figure 1, demonstrates the crystallization of metallic liquid. The inflection point determines the crystalline temperature  $T_c$ , being 1090 K at the pressure of 12 GPa and 1190 K at the pressure of 20 GPa. The slope of crystallization temperature versus pressure is clearly altered as compared with that of the glass transition temperature versus pressure, having a rate of  $6.4 \text{ K GPa}^{-1}$ , presented in figure 2. The value is comparable with the known data,  $1.5 \text{ K GPa}^{-1}$  for Zr-based BMG at a heating rate of  $0.3 \text{ K min}^{-1}$  [4]. The larger decrease of volume under higher pressure makes the atomic diffusion distance shorten more noticeably, which favours the formation of crystalline solid.

Further evidence supporting above conclusion is the PCF. Two quenching process performed on the EAM NiAl liquid under the two pressures (namely 10 and 20 GPa), as measured by the temperature dependence of PCF, are presented in figure 3. For comparison, the PCFs for NiAl alloy at 0 GPa are also analysed. The obvious splitting of the second peak of

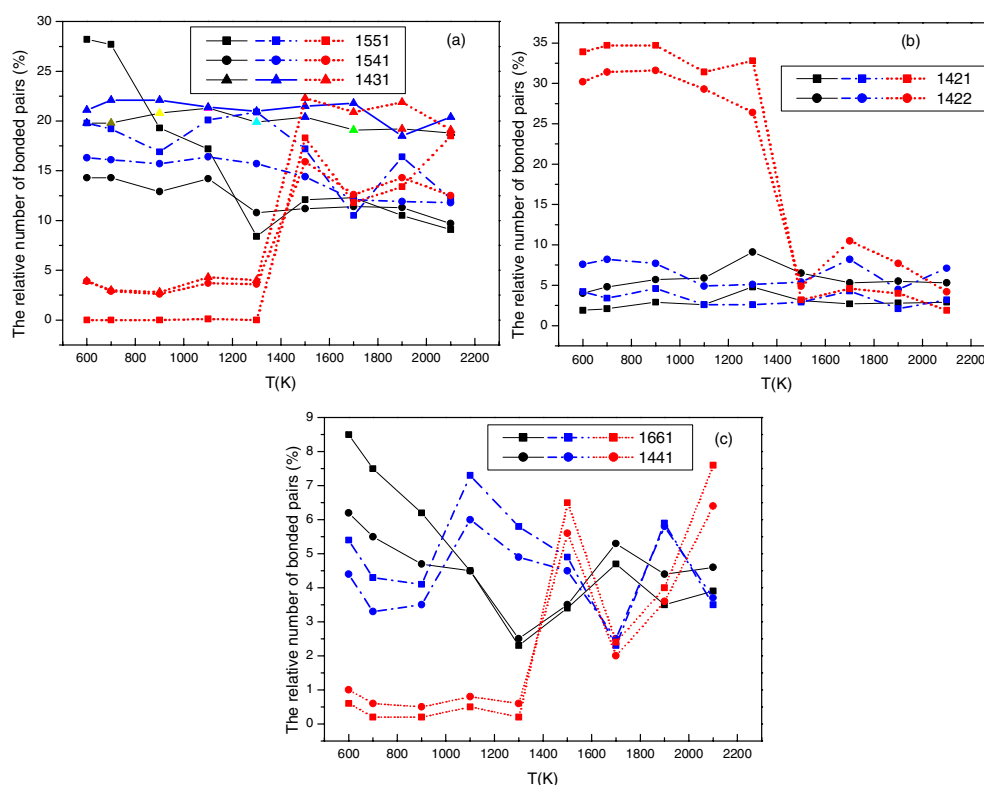


**Figure 2.** The glass transition temperature and crystallization temperature as a function of pressure. The glass transition temperature increases significantly with increasing pressure, compared with the crystallization temperature versus pressure. It also shows that the critical pressure to form metallic glass is 10 GPa at a cooling rate of  $2 \text{ K ps}^{-1}$ . The data are linearly fitted as solid lines.



**Figure 3.** Pair correlation functions for several temperatures. Solid lines are simulation data at 0 GPa, short dotted lines are simulation data at 10 GPa, short dashed lines correspond to simulation results at 20 GPa.

$g(r)$  gives strong evidence of an amorphous structure at 0 GPa. The shape of the PCF curves at 10 GPa is similar to that at 0 GPa, except that the first peak becomes more pronounced in magnitude at the same temperature, and the corresponding position of the first maximum in the PCF curve exhibits a slight inward shift as pressure is applied in the liquid. The shift of the PCF



**Figure 4.** The bonded pairs selected as a function of temperature. Solid lines are the simulation data at 0 pressure; short dotted lines correspond to the results at 10 GPa; short dashed lines are the simulation result at 20 GPa. (a) 1551, 1541, 1431; (b) 1421, 1422; (c) 1441, 1661.

means that high pressure causes the atomic nearest-neighbour distance, which is commonly used to scale the size of the atom cluster in the liquid, to shorten. That is to say, the size of atom cluster becomes smaller compared with that at 0 GPa. In contrast to that at 10 GPa, an increase in pressure (20 GPa, short dashed lines in figure 3) alters the atomic nearest-neighbour distance little, suggesting that the nearest-neighbour distance between atoms is not sensitive to higher pressure; this agrees well with the simulation result of liquid germanium based on the tight-binding potential [17]. There are weak sharp crystalline peaks appearing on the broad peak with the decreasing of temperature, and occurrence of typical crystalline peaks is obvious at lower temperature, indicating the existence of crystals with relatively regular crystal lattice structure. These changes suggest that different pressures could cause different microstructures, which have influences on the macro-properties of materials.

In order to obtain more detailed information on the liquid, the PA technique is used to characterize the microstructure in the system. Results for various typical bonded pairs under the three pressures are reported in figure 4. Figure 4(a) indicates that the number of 1551, 1541 and 1431 bonded pairs corresponding to an icosahedral cluster increases rapidly as the temperature drops. The number of 1551 bonded pairs makes up 9.1% of all kinds of bonded pairs in the melts; with decreasing temperature, the number of 1551 bonded pairs reaches the maximum value of 28.2% at a temperature of 600 K, occupying a predominant position in the system, which indicates that the liquid is inclined to the amorphous state at 0 GPa. This is



consistent with the fact that the second peaks of the PCF split into two sub-peaks. The number of 1431 bonded pairs changes little, from 18.8% in the liquid to the 19.8% in the glass at 0 GPa. The number of 1551 and 1541 bonded pairs at 10 GPa increases on the whole with the decrease of temperature and reaches its maximum value at a temperature of 1100 K, nearly close to its glass transition temperature (1050 K). Its total amount is smaller than that at 0 GPa, due to the fact that the high pressure restricts the diffusion of atoms at a rapid cooling rate, and more liquid structure has been kept. At the pressure of 20 GPa, in contrast, the number of 1551, 1541 and 1431 bonded pairs decreases sharply at a temperature of 1300 K during the cooling process, and they almost disappear at lower temperature. We can make a conclusion that the disorder structure representing the icosahedral cluster is discarded in the competition processing at 20 GPa: the three bonded pairs decompose and transform into other bonded pairs in favour of more stable structures.

Figure 4(b) presents the temperature dependence of the number of 1421 and 1422 bonded pairs which represents hcp-type structures under the different pressures. It is found that the relative numbers of 1421 and 1422 bonded pairs remain unchanged at 0 GPa and at 10 GPa within the temperature range 500–2100 K. However, one striking feature observed in figure 4(b) is that the numbers increase rapidly as the temperature falls below 1500 K at 20 GPa, making up more than 70% of all kinds of bonded pairs at low temperature, which indicates that the liquid crystallizes into crystals with hcp-type structure although the solid NiAl belongs to the B2-type crystal lattice structure. It embodies the feature of structural variation between the melt and solid under the control of external pressure.

Figure 4(c) indicates that the number of 1441 and 1661 bonded pairs representing bcc-type structures increases with the decrease of temperature when the temperature is below 1300 K at 0 GPa. At a pressure of 10 GPa, however, the numbers of the two bonded pairs remain unchanged during the whole cooling process. The results show that, despite the formation of glass, the clusters in metallic glass are various, embodying the diversity in the structure of glassy materials. It is interesting to note that the number of 1441 and 1661 bonded pairs drops sharply when the temperature is below 1300 K at 20 GPa; the total number is no more than 2%, which is inconsistent with the fact that NiAl has the B2-type structure. The external pressure makes the melt's structure change greatly, which gives rise to the differences of solidification products.

An isostructural phase transition occurs in the Al-rich Ni–Al alloys [24]. The pressure–temperature phase diagram for  $\text{Ni}_{1-x}\text{–Al}_x$  alloys at different  $x$  has been presented and it indicated phase-coexistence lines. The region below the line corresponds to the vacancy-rich solid solution and that above the line to antisite-rich solid solution. The driving force for this phase transition is the positive defect mixing enthalpy originating from elastic interaction between vacancies and antisites on the Ni sublattice. No phase-coexistence lines have been found in our simulation. When low pressure (less than 10 GPa) is applied to the liquid, the glass-forming ability increases with the increasing pressure: the number of 1551 and 1541 bonded pairs representing the icosahedral cluster plays a very important role in the glass formation, while higher pressure (10–20 GPa) causes the formation of crystals with hcp-type structure. This seems to be incompatible with the simulation results above. The effect of pressure on the solidification is complicated. Generally, a pressure applied to the metallic liquid might have two effects: the first effect is the suppression of atomic diffusion in the liquid, which promotes the formation of glass; the second effect of applying pressure on the liquid is densification by reducing the free volume of liquid, which favours the formation of crystalline solid. Therefore, the influence of pressure on the vitrification and crystallization of metallic liquid is mainly governed by the competition process of the two factors. Not only does a decrease of volume in the liquid occur, but also the atomic diffusion is retarded by

the applied pressure. Under lower pressures (less than 10 GPa in our simulations), the free volume in the liquid is relatively larger than that under higher pressure at the same temperature, and the suppression of the atomic diffusion becomes more prominent in the liquid. Since the crystallization process is accompanied by long-range atomic diffusion processes, a long time would be needed if the system becomes crystalline solid. The suppression of atomic diffusion in a wide range, due to high cooling rate, promotes glass formation. With increasing pressure (10–20 GPa in our simulations), the decrease of volume is more obvious, and it plays a predominant role in the solidification process, shortening the atomic diffusion distance, thereby making atomic diffusion in a relatively small range possible. It should be noted that all crystallization temperatures we simulated are higher than glass transition temperature, indicating that atomic diffusion in a wide range is developed in the supercooled liquid region with a relative higher temperature, susceptible to the nucleation of crystals, and as a result, higher crystallization temperatures are achieved. Detailed structural analysis indicates that the system crystallizes at 20 GPa.

## 5. Conclusion

The effect of pressure on the vitrification and crystallization behaviours of liquid NiAl has been investigated by molecular dynamics simulation. It is concluded that the applied pressure strongly affect the vitrification and crystallization processes of the metallic liquid. Various clusters play an important role in the transition from liquid to solid. At low pressure (less than 10 GPa), the icosahedral order detected by evaluating 1551 bonded pairs increases at the glass transition temperature, suggesting the formation of a glassy state at 0 GPa, while the fact that number of the 1551 bonded pairs at a pressure of 10 GPa is lower than that at 0 GPa is due to the suppression of atomic diffusion in the liquid. Our simulation further reveals that the number of 1421 and 1422 bonded pairs representing hcp-type clusters is in a predominant position in the formation of crystals at 20 GPa. The shortness of the average near-neighbour distance between atoms is not obvious as external pressure is applied in the melt. The glass transition temperature increases with pressure within the range 0–10 GPa; meanwhile, the crystallization temperature still increases with pressure, at a rate of  $6.4 \text{ K GPa}^{-1}$ . The vitrification and crystallization processes in supercooled liquid under various pressures are governed by the competition process of the densification and the suppression of atomic diffusion in the liquid.

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