Research Article

Molecular Dynamics Simulation of Solidification of Pd-Ni Clusters with Different Nickel Content

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Molecular dynamics simulation has been performed for investigating the glass transition of Pd-Ni alloy nanoparticles in the solidification process. The results showed that the Pd-Ni nanoparticles with composition far from pure metal should form amorphous structure more easily, which is in accordance with the results of the thermodynamic calculation. There are some regular and distorted fivefold symmetry in the amorphous Pd-Ni alloy nanoparticles. The nanoclusters with bigger difference value between formation enthalpies of solutions and glasses will transform to glass more easily than the other Pd-Ni alloy nanoclusters.

1. Introduction

In the past decades, because of the high special surface area and its excellent catalytic performance, pure metal or its alloy nanoparticles have been studied and used widely in catalytic chemistry [1–4]. It is well known that the structure of nanocatalyst particle affects the catalytic activity and selectivity evidently. However, in most experimental cases some restricted conditions were required normally, which blocks the studies on nanostructure of catalyst profoundly. As an economical research method, the computer simulation of molecular dynamics (MD) has been applied to study the metal cluster structure or properties by many researchers successfully [5–11].

Considering the structure stability of catalyst nanoparticles, many MD simulations have been done for researching the melting process of the metal clusters [8–11]. Nevertheless, there are few studies about structure transformation in solidification of the melted clusters. The atomic configuration, which affects the catalyst efficiency, should be different with altering the atomic ratio in the clusters or the solidification process.

Pd-Ni alloy clusters, synthesized by many methods, have been used as catalyst in many reactions, especially in hydrogenation [1]. The melting and solidifying process of Pd-Ni

nanoparticles will occur in some preparation or application, such as supporting the cluster on the carbon nanotubes or other catalytic reactions. Therefore, the solidification of melted Pd-Ni nanoparticles has been simulated by molecular dynamics in the present work, and the tendency to forming noncrystalline structure of Pd-Ni alloy with different element content has been also studied here by thermodynamic calculation method.

2. Method of Simulation

The parallel code LAMMPS was used for all MD simulations in this work [12]. The embedded-atom method (EAM), a set of n -body potentials, has been proved to accurately describe various dynamic properties of transition and noble metals. The EAM potential data used here was obtained from the literature [13]. The Newtonian equations of motion are integrated using the Verlet method with a time step of 5×10^{-4} ps.

The calculation is performed in two steps. Firstly, the melting models for simulating solidification process were obtained after the initial models were heated to 2300 K and relaxed enough time (50 ps). Then, the melting models were subjected to cooling process consisting of a series of dropping

TABLE 1: Content of nickel of every cluster model.

Model	Ni (at.%)	Model	Ni (at.%)
Pd	0	Ni800	58.3
Ni200	14.6	Ni1000	72.9
Ni400	29.2	Ni1200	87.5
Ni600	43.7	Ni	100

and keeping temperature MD simulations with temperature decrements of 100 K. The cooling rate of 4 K/ps and the equilibration simulation time of 10 ps were used in the present study. The cooling process of nanoclusters was simulated with constant temperature and constant volume (NVT) molecular dynamic in enough large box with a periodic boundary condition.

The initial models with 1372 atoms (diameter about 2 nm) started with geometries constructed from a FCC block of Pd. Through replacing the Pd atom with Ni atom randomly, the alloy models with different nickel atom content can be created. The exponent of all models can be found in Table 1.

The radial distribution function (RDF) shown as in (1), being regarded as one of the most important parameters, is used to describe the structure characterization of solid, amorphous and liquid states [14]. Consider

$$g(r) = \frac{\Omega}{N^2} \cdot \left\langle \frac{\left(\sum_{i=1}^{N_i} n_i \right)}{4\pi r^2 \Delta r} \right\rangle, \quad (1)$$

where $g(r)$ is the probability of finding an atom in a distance ranging from r to $\Delta r + r$ (Δr is the step of calculation), Ω is the simulated volume of unit cell, N is the number of atoms in the system, and N_i is the average number of atoms around the i th atom in the sphere shell ranging from r to $r + \Delta r$.

Besides MD simulation, Miedema's thermodynamic theory was used for calculating the forming energies of binary transition metal alloy system, which can explain the glass-forming ability of Pd-Ni alloy with different Ni content. On the basis of Miedema's thermodynamic theory [15–19], the formation enthalpy of Pd-Ni solid solution is expressed as

$$\Delta H_{\text{PdNi}} = \Delta H_{\text{PdNi}}^{\text{chem}} + \Delta H_{\text{PdNi}}^{\text{eles}} + \Delta H_{\text{PdNi}}^{\text{stru}}, \quad (2)$$

where $\Delta H_{\text{PdNi}}^{\text{chem}}$ results from the electronic redistribution occurring when the alloy forms, $\Delta H_{\text{PdNi}}^{\text{eles}}$ is the size-mismatch contribution to the formation enthalpy in a binary system, and $\Delta H_{\text{PdNi}}^{\text{stru}}$ accounts for the difference in valence and crystal structure of the component metals. However, the structure of palladium is close to that of nickel. That is to say, the $\Delta H_{\text{PdNi}}^{\text{stru}}$ can be ignored here.

Then the Gibbs free energy of Pd-Ni solid can be expressed as

$$\Delta G_{\text{PdNi}} = \Delta H_{\text{PdNi}}^{\text{chem}} + \Delta H_{\text{PdNi}}^{\text{elec}} - T \cdot \Delta S_{\text{PdNi}}^{\text{ideal}}, \quad (3)$$

where $\Delta S_{\text{PdNi}}^{\text{ideal}}$ is the ideal mixing entropy. Consider

$$\Delta S_{\text{PdNi}}^{\text{ideal}} = X_{\text{Pd}} \cdot \ln X_{\text{Pd}} + X_{\text{Ni}} \cdot \ln X_{\text{Ni}},$$

$$\Delta H_{\text{PdNi}}^{\text{chem}} = X_{\text{Pd}} \cdot X_{\text{Ni}}$$

$$\cdot (f_{\text{NiPd}} \cdot \Delta H_{\text{NiinPd}}^{\text{amp}} + f_{\text{PdNi}} \cdot \Delta H_{\text{PdinNi}}^{\text{amp}})$$

$$f_{\text{NiPd}} = X_{\text{Pd}}^S \cdot \left[1 + K_r \cdot (X_{\text{Pd}}^S \cdot X_{\text{Ni}}^S)^2 \right], \quad (4)$$

$$f_{\text{PdNi}} = X_{\text{Ni}}^S \cdot \left[1 + K_r \cdot (X_{\text{Pd}}^S \cdot X_{\text{Ni}}^S)^2 \right],$$

$$X_{\text{Pd}}^S = \frac{X_{\text{Pd}} \cdot V_{\text{Pd}}^{2/3}}{X_{\text{Pd}} \cdot V_{\text{Pd}}^{2/3} + X_{\text{Ni}} \cdot V_{\text{Ni}}^{2/3}}, \quad X_{\text{Pd}}^S + X_{\text{Ni}}^S = 1,$$

where X_{Pd} , X_{Ni} , V_{Pd} , and V_{Ni} are the mole ratio and atomic volume of Pd and Ni, respectively. The factor K_r takes the values 8, 5, and 0 for intermetallics, metallic glasses, and solid solutions, respectively; $\Delta H_{\text{NiinPd}}^{\text{amp}}$ is given by

$$\Delta H_{\text{NiinPd}}^{\text{amp}} = \frac{2V_{\text{Ni}}^{2/3}}{\left[(n_{\text{WS}}^{1/3})_{\text{Ni}}^{-1} + (n_{\text{WS}}^{1/3})_{\text{Pd}}^{-1} \right]} \cdot \left\{ -P \cdot (\phi_{\text{Ni}} - \phi_{\text{Pd}})^2 + Q \cdot \left[(n_{\text{WS}}^{1/3})_{\text{Ni}} - (n_{\text{WS}}^{1/3})_{\text{Pd}} \right]^2 - R \right\}. \quad (5)$$

The parameters, such as P , Q , and R , were shown in Table 2. The $\Delta H_{\text{PdNi}}^{\text{amp}}$ can also be calculated by this kind of formula.

Similar to the form of $\Delta H_{\text{PdNi}}^{\text{chem}}$, the $\Delta H_{\text{PdNi}}^{\text{eles}}$ can be expressed as

$$\Delta H_{\text{PdNi}}^{\text{eles}} = X_{\text{Pd}} \cdot X_{\text{Ni}} \cdot (X_{\text{Pd}} \cdot \Delta H_{\text{NiinPd}}^{\text{eles}} + X_{\text{Ni}} \cdot \Delta H_{\text{PdinNi}}^{\text{eles}}),$$

$$\Delta H_{\text{NiinPd}}^{\text{eles}} = \frac{2K_{\text{Ni}} \cdot \tau_{\text{Pd}} \cdot (V_{\text{Ni}} - V_{\text{Pd}})^2}{3K_{\text{Ni}} \cdot V_{\text{Pd}} + 4\tau_{\text{Pd}} \cdot V_{\text{Ni}}},$$

$$\Delta H_{\text{PdinNi}}^{\text{eles}} = \frac{2K_{\text{Pd}} \cdot \tau_{\text{Ni}} \cdot (V_{\text{Ni}} - V_{\text{Pd}})^2}{3K_{\text{Pd}} \cdot V_{\text{Ni}} + 4\tau_{\text{Ni}} \cdot V_{\text{Pd}}}, \quad (6)$$

where K_{Ni} and K_{Pd} are bulk moduli of Ni and Pd, respectively, τ_{Ni} and τ_{Pd} are shear moduli of Ni and Pd, respectively.

The Gibbs free energy of formatting amorphous Pd-Ni alloy is

$$\Delta G_{\text{PdNi}}^{\text{amor}} = \Delta H_{\text{PdNi}}^{\text{chem}} - T \cdot \Delta S_{\text{PdNi}}^{\text{ideal}} + X_{\text{Ni}} \cdot \Delta G_{\text{Ni}}^{a-s} + X_{\text{Pd}} \cdot \Delta G_{\text{Pd}}^{a-s}. \quad (7)$$

The $\Delta G_{\text{PdNi}}^{\text{amor}}$ contains the free energy of the mixing of the pure liquid metals (the first two terms) plus the free energy difference between the amorphous state and the crystalline state of the pure components. The difference can be expressed as

$$\Delta G^{a-s} = \Delta H_m^i \cdot \left[\frac{(T_m^i - T)}{T_m^i} \right] \cdot \left[\frac{2T}{(T_m^i + T)} \right], \quad i = \text{Pd or Ni}, \quad (8)$$

TABLE 2: Parameters for calculating forming energy of Pd-Ni binary alloy [24–26].

	T_m (K)	ΔH_m (kJ/mol)	P	Q/P	R/P
Pd	1828.0	16.74	14.2	9.4	14.2
Ni	1728.3	17.48			
	Φ (volt)	$V^{2/3}$ (cm ²)	$N_{WS}^{1/3}$ (d.u.)	K (GPa)	τ (GPa)
Pd	5.45	4.29	1.67	183.3	43.5
Ni	5.2	3.52	1.75	193.0	83.9

FIGURE 1: Total energy versus temperature curve for Pd-Ni clusters during cooling process.

where the ΔH_m is the molar heat of fusion, T_m is the melting points of metal.

For Pd-Ni cluster, surface energy should be considered in the forming energy. For the same size of the clusters and simplifying calculation, the surface energies of noncrystalline and crystalline clusters were considered as equal approximately. Then the term of surface energy was neglected in this study.

3. Results and Discussion

When liquid nanocluster translates to crystal cluster, the jump should appear in caloric curve. However, the cluster only has 1372 atoms, which leads to less energy decrease as crystallization. Therefore, the visible jump is not found in the Figure 1.

Figure 2 shows the radial distribution function (RDF) curves of Pd-Ni alloy clusters at 300 K. Crystalline states are visible through the well-defined peaks, which represent positions of the first, second, third, and n th nearest neighbor atoms. It proves the presence of an FCC crystal structure in Pd, Ni200, Ni1200, and Ni models. Because of the equilibrium distance of Pd atom bigger than that of Ni, the Pd atom content increasing, the first neighbor distance generally increasing, which is found in Figure 2. For Ni400, Ni600,

FIGURE 2: Radial distribution function (RDF) of Pd-Ni clusters at 300 K with the cooling rate of 4 K/ps.

Ni800, and Ni1000 clusters, the number of the first neighbor atoms is fewer than that of Pd, Ni200, Ni1200, and Ni, while the splitting of the second peak, denoted in Figure 2 by single arrow line, appears in the RDF curves of Ni400, Ni600, Ni800, and Ni1000 clusters. The splitting of the second peak is a well-known characteristic feature of solid amorphous structure of metallic glass, and the number of the first neighbor atoms is fewer, which can effectively describe the characteristics of the geometric structural evolvement [20–22].

Pair analysis (PA) technique, which can effectively describe the characteristics of the geometric structural evolvement, was used for the analysis of the geometric features of the atomic cluster [20–22]. In this study, PA method was used to analyze the structural changes accompanying the solidification process of melting Pd-Ni clusters. Based on the regulation of bond pair, two atoms are within a specified cutoff distance of each other and they are called a bonded pair of clusters [22, 23]. In RDF curves, if $g(r_c)$ is the first minimum value, then r_c was defined as cutoff distance for PA. Four-index number $ijkl$ is used to express bonded pairs of atomic clusters by Honeycutt and Andersen [20]. If any atomic pair A-B forms a bond, $i = 1$ and otherwise $i = 2$; j refers to the number of near neighbors which form bonds with both atom A and atom B; k stands for the number of pairs among the neighboring atoms forming bonds; l is a special distinguished index parameter. Based on the PA technique, the 1201 and 1311 bond pairs represent

FIGURE 3: Continued.

FIGURE 3: Relative amount of various atomic-bonded pairs includes (a) 1201, (b) 1311, (c) 1321, (d) 1421, (e) 1422, (f) 1551, (g) 1541, and (h) 1431 in Pd-Ni clusters at different temperatures during cooling.

the rhombus symmetrical features of short-range order. The FCC structure has the type of 1421 bond pairs, whereas the HCP crystal has the equal number of 1421 and 1422 bond pairs. The difference between 1421 and 1422 bond pairs is the topological arrangement of the two bonds between the four neighbors. The bond pair 1551, corresponding to a pentagonal bipyramid, is the characteristic of icosahedral order.

Figure 3 shows the normalized abundance of selected pairs and polyhedra in the Pd-Ni clusters simulation in the present study. The results indicate that the number of the 1201, 1311, 1321, 1421, 1422, 1551, 1541, and 1431 pairs will change with temperature dropping, especially when the temperature lower than 1000 K. Because all the clusters are in the liquid state at high temperature, the 1201 and 1311 pairs with relative high proportion shown in Figures 3(a) and 3(b), indicating short-range order structure, exist in all the clusters. According to the case of proportion of every type pair, all the clusters calculated in present work can be assorted into two kinds. The change tendency of the Ni, Ni1200, Ni200, and Pd, labeled with the first type, is different with the second type clusters including Ni400, Ni600, Ni800, and Ni1000. With the temperature dropping, solidification process leads to the proportion of 1201 pairs in all Pd-Ni clusters decreasing gradually. For the first type clusters, the proportion of 1421 and 1422 pairs increased observably to the relative high value shown in Figures 3(c) and 3(d), which indicates that most atoms in Ni, Ni1200, Ni200, and Pd are arranged mainly as FCC or HCP structure. And this result is in accordance with characteristic peaks shown in Figure 3. There are also 15–20% 1311 pairs in the first type clusters due to the surface atoms packing for the small surface energy. It can estimate the crystalline point where the 1421 pair number is evaluated abruptly. And the crystalline temperature of Ni, Ni1200, Ni200, and

Pd nanoclusters was about 800 K, 700 K, 600 K, and 800 K, respectively.

Relative amount of various bonded pairs in the second type Pd-Ni clusters was different from that of the first kind of clusters. In these clusters, the notable increase of 1311, 1321, 1551, 1541, and 1431 pairs was presented as the temperature dropping took place. These results suggested that the main atom structure of the second Pd-Ni clusters was short-range order at low temperature; namely, Ni400, Ni600, Ni800, and Ni1000 clusters are in amorphous states. In addition, the three types of pairs (1551, 1541, and 1431) corresponding to inherent structures with regular and distorted fivefold symmetries account for about 25% of all pairs, which implies that part of short-range order is local icosahedral order, meaning the order characteristic of a 13-atom icosahedron. There is also small proportion of 1421 and 1422 bond pairs in the second type clusters which indicates that crystalline short-range order exists in the disorder system [20, 21].

The results of MD simulation, which indicate that the clusters were easier to form amorphous structure when the number of Pd was close to that of Ni atom, can also be explained by thermodynamic calculation. Figure 4(a) shows the formation enthalpies of glasses (ΔG^{amor}) and solutions (ΔG^{cry}) of Pd-Ni alloy clusters calculated by the Miedema's model [16]. It is commonly regarded that the alloys could be vitrified into glass more easily only when the enthalpies of glasses are bigger than those of solution. So the compositions of a possible amorphous structure former should be ranging from about Pd75Ni25 to Pd28Ni72, being marked by dash line in Figure 4(a). In this composition region, the difference value between formation enthalpies of solutions and glasses has been used for expressing the glass formation ability (GFA) of Pd-Ni alloy clusters.

FIGURE 4: The formation enthalpies as function of the composition of Ni.

Evidently, in the curve of $\Delta G^{\text{cry}} - \Delta G^{\text{amor}}$ versus nickel atom content, shown in Figure 4(b), the cluster with about 50 percent of nickel can form glass more easily than other clusters. More leaving away from this composition point the value of the difference is much smaller, which suggested that the GFA increases firstly and then decreases with more nickel atoms in the cluster. For the verification of this law, the slower cooling process, in which the cooling rate was 0.8 K/ps and the equilibration simulation time was 100 ps, has also been used to simulate solidification of Pd-Ni alloy clusters. Figure 5 shows that the Pd, Ni200, Ni1200, and Ni clusters were presenting more perfect crystal structure and Ni1000 cluster showed the crystalline structure after the solidification process with slower cooling rate.

4. Conclusion

In summary, the solidification of Pd-Ni clusters with different nickel content has been studied in the present work. The results of molecule dynamic simulation and thermodynamic study certified that Pd-Ni clusters with composition close to 50 at.% will form noncrystal structure more easier than other Pd-Ni clusters.

Conflict of Interests

The authors declare that there is no conflict of interests regarding the publication of this paper.

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FIGURE 5: Radial distribution function (RDF) of Pd-Ni clusters at 300 K with the cooling rate of 0.8 K/ps.

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