About Structural Transition of Nickel Metal

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Abstract. A molecular dynamics (MD) simulation study has been performed to investigate the structural transition of nickel metal using Pak-Doyama potential. The local atomic structure was analyzed through the radial distribution function (RDF), coordination number distribution and 3D visualization. It was shown that the splitting of RDF second peak appears when the liquid transforms to amorphous solid. We found that the liquid state contains a significant amount of nano-crystalline nucleations, which strongly depends on the temperature and MD time steps. Accordingly, the simulation shows that the crystallization is originated from expanding of nano-crystalline nucleations.

Keywords: MD simulation, nickel, nano-crystalline nucleation, liquid and amorphous.

1. Introduction

The structure and atomic mechanism of glass formation from liquid metal has been found from intensive study from both experiment and computer simulation. By using different diffraction techniques as X-ray and neutron diffraction or turning electronic microscopic, experiment data has provided the important information of structural general arrangement of metals through the RDF and structure factor. Both functions have splitting second peak, which was usually thought to be related to the existence of local icosahedral in amorphous state [1-7]. However, the atomic mechanism of amorphous formation from liquid state is still not well understood. This is one of problems, which is interested in the present work. In addition, our understanding of the atomic mechanism in crystalline and liquid states are still limited. MD simulation study showed that during solidification of aluminum, a crystalline and amorphous like-structure is formed, depending on the cooling rate [8-9]. However, the atomic mechanism of crystallization from liquid metal has not yet been fully investigated.

Therefore, the main purpose of this paper is to indicate the atomic mechanism of crystallization and amorphous formation in nickel metal using the pair RDF, coordination number distribution and 3D visualization. The paper is organized as follow: After a brief introduction, we describe in details the simulation technique in section 2. The structural

characteristics, crystallization and amorphous formation are presented in section 3. Section 4 is devoted to the main conclusions.

2. Calculation procedure

We consider a system of single-component atoms that interact mutually through the Pak–Doyama potential [10-12]:

$$U\left(r_{ij}\right) = -0.12929\left(r_{ij} - 1.82709\right)^4 + 1.16473\left(r_{ij} - 2.50849\right)^2 - 0.135705; \; r_{ij} < \; 3.44 \; \text{Å} \qquad (1)$$

Here r_{ij} is inter-atomic distance in Å and $U(r_{ij})$ in eV. We performed the simulation in a cube containing 4394 particles under periodic boundary conditions. The equations of motion were solved numerically using the Verlet algorithm. Initial random configuration was equilibrated at constant amorphous density of 7.91 g/cm^3 by relaxation for 10^6 MD steps at temperature of 5000 K (i.e. NVT ensemble). From this melt we prepare eight other samples at temperature: 1379.97, 1167.05, 994.60, 873.58, 642.10, 516.33, 334.59 and 118.28 K. Then each sample obtained was relaxed for 4×10^6 MD step which is equal to 0.4 fs. The relaxation is continued until the system reaches equilibrium state.

3. Results and discussion

Fig.1 shows the structural characteristics of our model, which meets the experimental data [2-4]. RDF also has a splitting second peak like that observed in practice, which was often thought to be related to the existence of icosahedrals in the amorphous system. Fig.2 shows the RDFs obtained at different temperatures for liquid and amorphous samples. We can be seen that the height of RDF first peak increases with decreasing the temperature, so it follows that the nearest neighboring coordination is raised during solidification of material. Further, the positions of PRDF first peak and first minimum are almost unchanged with temperature. They locate at 2.55 and 3.40 Å, respectively. At high temperature, in the temperature range 1379.97-994.60 K, RDF shows a shape typical of normal liquid. It should be noted that below 873.58 K the RDF form closes the RDF of metal nano-cystal. When the temperature is reduced at 642.10 K, the second peak of RDF is split which shows the transition from the nano-crystal to amorphous state. The splitting of RDF second peak is also observed by other

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researchers for different materials. This result was considered as a common feature of amorphous matter [2,3,12]. This fact can be also seen from the distribution of coordination number in Fig. 3. At 873.58 K, the mean coordination number is 14, which is also coordination number of bcc and fcc nickel nano-crystal (weak crystalline structure). On the other hand, down 642.10 K the mean coordination number is 13 and it is 12 for models in the temperature range 1379.97-994.60 K. These values are in good agreement with the coordination number of amorphous and liquid states. From above discussion, one can see that there are three different states of nickel metal, i.e., amorphous, nano-crystal and liquid states in the temperature range 118.28-1379.97 K.

To determine the glass and amorphous transition temperature (T_g and T_a) in MD simulations we use the Wendt–Abraham ratio defined as g_{min}/g_{max}. Here g_{min} is first minimum value and g_{max} is first maximum value of RDF. The ratio g_{min}/g_{max} at different temperatures is calculated and the obtained data plotting versus temperature is shown in Fig.4. From this figure the temperature T_g, T_a are obtained near 994.60 and 642.10 K, respectively. One can be seen that the existence of different phases can be detected on the base of Wendt-Abraham ratio.

Next, we focus on the question of the atomic mechanism of nano-crystalline formation from liquid state. The three-dimensional (3D) visualization will be a useful tool to investigate the nano-crystalline formation for metal materials. Fig.5 presents the atom distribution in simulation box for liquid and crystalline states. At the temperature 873.58 K, atom arrangement is more homogenous (like-crystal) than high temperature models (see Fig. 5 a, b and c). This fact can be also seen from Fig. 5 d, e and f which present the atoms with the coordination number of 14. One can be seen that the atom with the coordination number of 14 significantly increases when the temperature decreases down below T_g. This result can be explained as follow, the liquid state must contain a significant amount of the nano-crystalline nucleations depending on the temperature and relaxation rate. It means that the temperature decreasing or appropriate relaxation rate accompanies with the expanding of nano-crystalline nucleations.

4. Conclusion

The structural analysis of nickel metal under temperature shows that the three different states of nickel can be detected on the base of Wendt-Abraham ratio. The simulation result indicates that the transition to amorphous state accompanies with the splitting of RDF second peak. A

distinctive result of this research is that the liquid state contains a significant number of nano-crystalline nucleations which plays a major role for crystallization process of metal systems.

Acknowledgments

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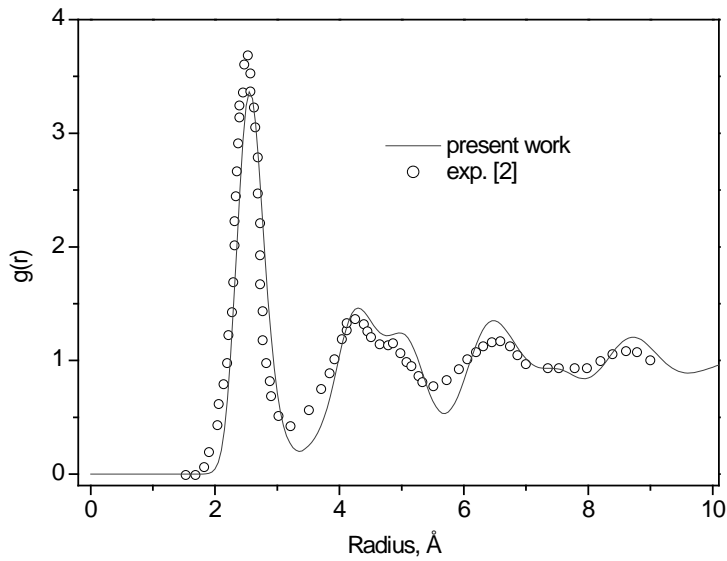12. Vo Van Hoang, Takashi Odagaki, The journal of physical chemistry B 20, (11page) (2010).

Fig. 1. The radial distribution function of the amorphous nickel model obtained at T = 334.59 K compared with the experimental X-ray [2].
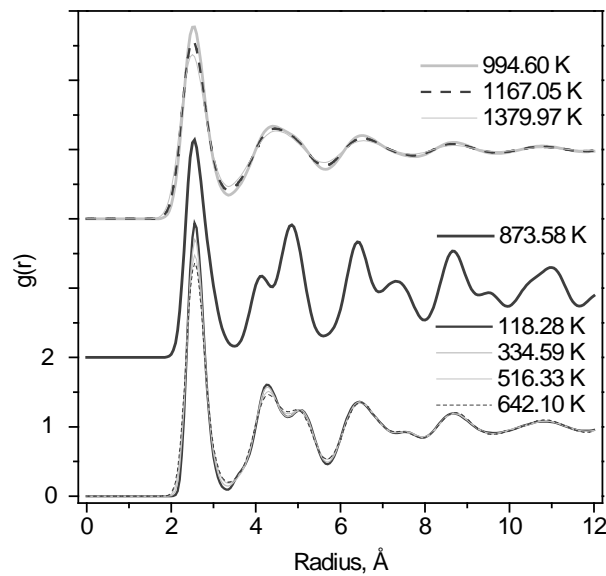

Fig. 2. The radial distribution functions for obtained nickel models at the different temperatures.
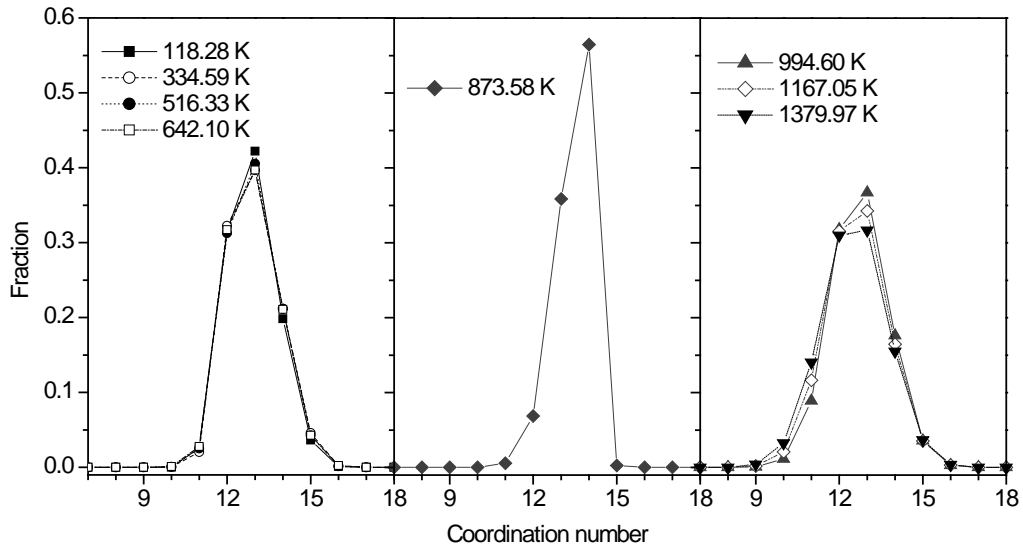
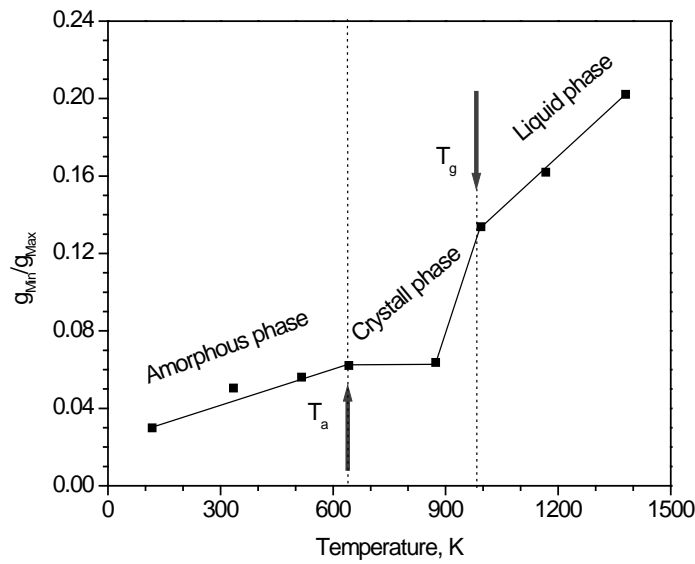**Fig. 3.** The coordination number distribution for nickel metal at the different temperatures.

Fig. 4. The temperature dependence of the g_{min}/g_{max} ratio for obtained models.

(a) 1379.97 K

(b) 994.60 K

(c) 873.58 K
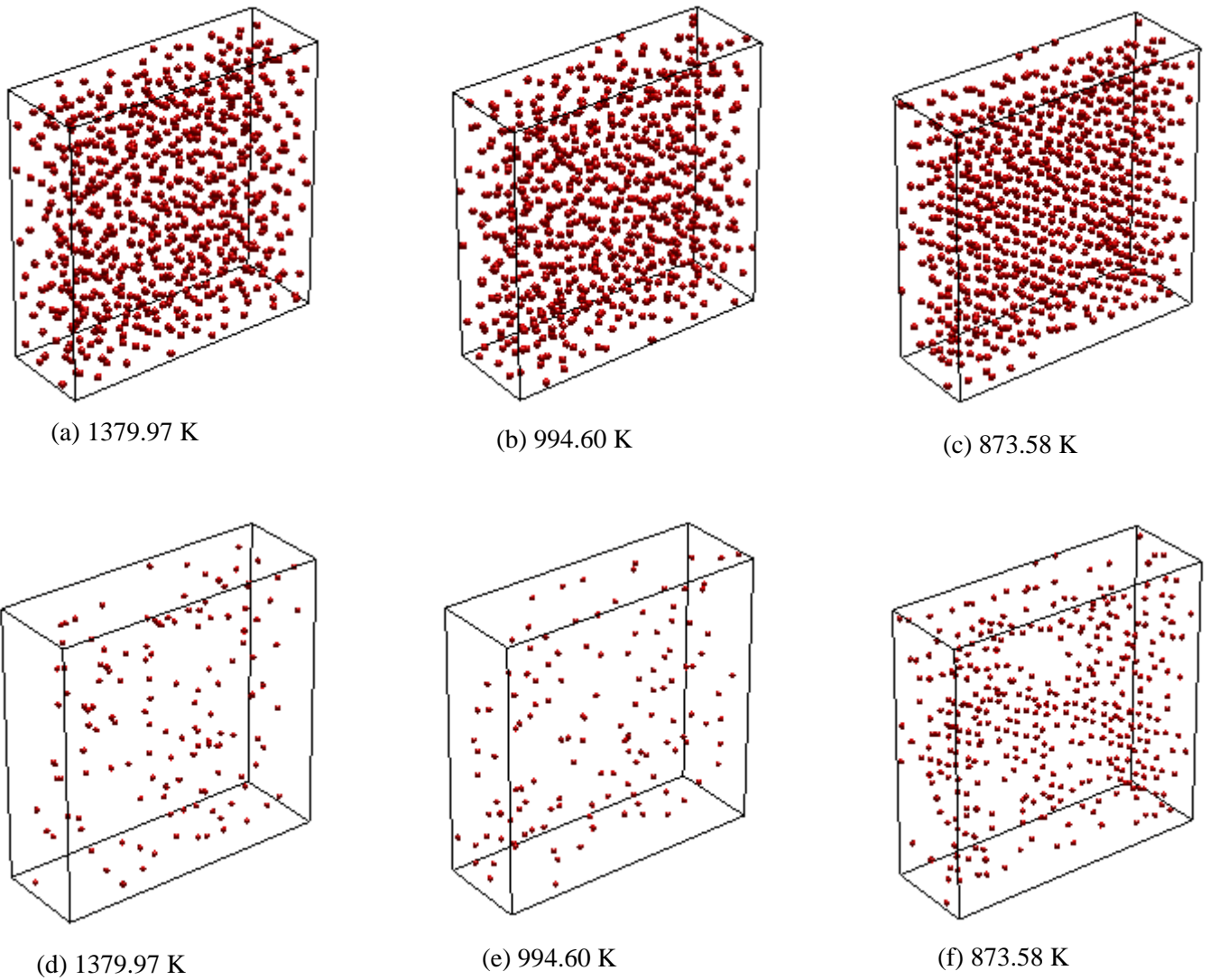
(d) 1379.97 K

(e) 994.60 K

(f) 873.58 K

Fig. 5. 3D visualization of nickel atoms arrangement for different temperature models: Here (a), (b) and (c) represent the atoms with coordination number of 13 and 14; (d), (e) and (f) represent the atoms with coordination number of 14.