Vol. **129** (2016) *ACTA PHYSICA POLONICA A* No. 3

Local Structural Features of Metallic Alloys: $Ni_{33}Zr_{67}$ and $Ni_{50}Zr_{50}$

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(Received January 26, 2016)

In this work we present the results of computer simulations molecular dynamics of the metallic alloys: $Ni_{33}Zr_{67}$ and $Ni_{50}Zr_{50}$. The critical glass-forming temperatures are defined from the behavior change of the Wendt–Abraham parameters of the studied systems. We have found that the increase in the concentration of nickel in the system NiZr leads to displacement of the critical glass-forming temperature in higher temperature region. It is shown that the structural transformations which were observed in the $Ni_{50}Zr_{50}$ system are not related with crystallization processes.

DOI: 10.12693/APhysPolA.129.293

PACS/topics: 61.20.Ja, 61.20.–p, 61.43.Fs

1. Introduction

The development and the production of new materials is an important activity in the continuous progress of science and technology. Amorphous metallic alloys with their unique physicochemical properties are one of such categories of advance materials that attract special interest of scientists and technologists [1–3]. So, for example, amorphous alloys which contain transition metals (Fe, Co, Ni) in the capacity of main component possess high tensile strength, that exceeds more than twice their crystal counterparts. Some of these amorphous alloys likewise possess high corrosion-resistance, excellent magnetic and electric properties [4]. All of these unique properties of amorphous metallic alloys are due to local disorder in the arrangement of atoms of the alloy [5, 6]. In this work we present the results of computer simulations molecular dynamics and structural analysis of amorphous metallic alloy, NiZr, as well as study of the influence of concentration dependence on the vitrification processes.

2. Details of simulation

Molecular dynamics study of the metallic alloys ($Ni_{33}Zr_{67}$ and $Ni_{50}Zr_{50}$) at different thermodynamical states and zero external pressure was performed.

The systems under study containing $N = 4000$ atoms were arranged in the cubic cells with the periodic boundary conditions. The interaction between atoms was carried out using the potential of interparticle interaction, proposed in Ref. [7]. Simulation was performed in the isothermal-isobaric ensemble (NpT). To maintain the system in thermodynamic equilibrium there were used the thermostat and barostat of Berendsen with an interaction parameter $\alpha = 10^{-14}$ s [8]. The cooling of the system was carried out in the isenthalpic-isobaric ensemble (NpH) with the cooling rate $\mathrm{d}T/\mathrm{d}t = 10^{13}$ K/s.

3. Results of simulation and discussions

Analysis of the structural peculiarities of metallic alloys was performed on the basis of calculation of the partial radial distribution function of particles in the system

$$g_{\alpha\beta}(r) = \frac{L^3}{N_\alpha N_\beta}\left\langle \sum_{j=1}^{N_\alpha} \frac{n_{j\beta}(r)}{4\pi r^2 \Delta r}\right\rangle, \quad \alpha,\beta \in \{Ni, Zr\}. \tag{1}$$

Here $g_{\alpha\beta}(r)$ is the probability of the atomic arrangement in the range from r to $r+\Delta r$, L — the length of edge of the simulation cell, N_α and N_β — the number of particles of type α and β, respectively. The value of $n_{j\beta}(r)$ determines the number of β-particles in a spherical layer with thickness of Δr on the distance r from the j-th particle. Figure 1 presents the temperature dependences of the radial distribution functions of particles, $g_{\alpha\beta}(r)$, calculated on the basis of computer simulations molecular dynamics. It was shown from Fig. 1 that system $Ni_{33}Zr_{67}$ with quenching completely transformed in amorphous state: the distribution function has a pronounced first peak and splitting of the second one. However, for the system $Ni_{50}Zr_{50}$ in the partial distribution functions for Zr–Zr pair there was observed the appearance of an additional extrapeak, which is located between first and second peaks, which characterizes, as a rule, the nucleation of a crystalline phase with a face-centered cubic (fcc) structure.

TABLE I

Translational order parameter $t_{\alpha\beta}$ in FCC lattice.

$Ni_{33}Zr_{67}$-system		$Ni_{50}Zr_{50}$-system	
Ni-Ni	1.848	Ni-Ni	1.870
Ni-Zr	1.788	Ni-Zr	1.871
Zr-Zr	1.757	Zr-Zr	1.870

To test this peculiarity we calculated the translational order parameter [9]:

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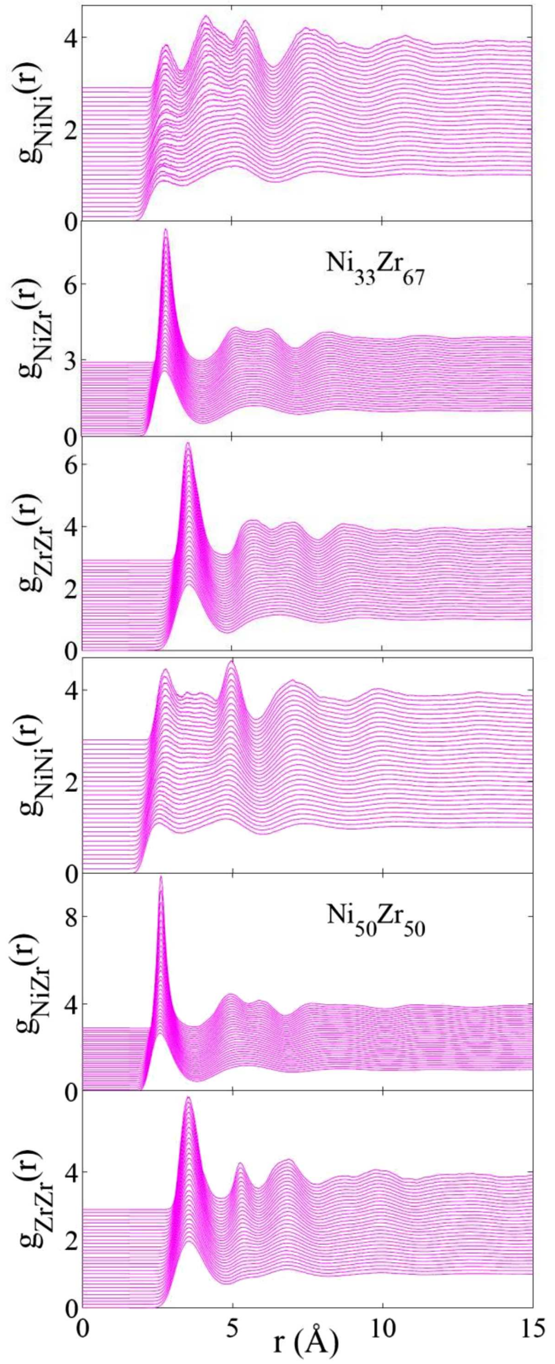

Fig. 1. Partial radial distribution functions of particles for $Ni_{33}Zr_{67}$-system (top panel) and $Ni_{50}Zr_{50}$-system (bottom panel).

$$t_{\alpha,\beta} = \frac{1}{r_M} \int_0^{r_M} |g_{\alpha,\beta}(r) - 1| \, \mathrm{d}r, \quad \alpha, \beta \in \{Ni, Zr\}, \quad (2)$$

values, which in the case of an ideal fcc-structure of the NiZr-system have been presented in Table I.

Figure 2 illustrates the temperature dependence of the translational order parameter for the different pairs (Ni–Ni, Ni–Zr, Zr–Zr). It is seen from the figure that with decrease of temperature the value of the parameter is increased, which indicates on the appearance of some translational ordering in the system. Even at very low temperatures ($T = 100$ K) the magnitude of the parameter takes very small values ($t \approx 0.20 \div 0.30$) as compared with the values for an ideal fcc lattice ($t \approx 1.70 \div 1.90$). This indicates on the high structural disorder of the particles regarding arbitrarily chosen direction (translation). The structural ordering in the system arises also due to local structural formation of atoms and can be characterized by the orientational order parameter [10]:

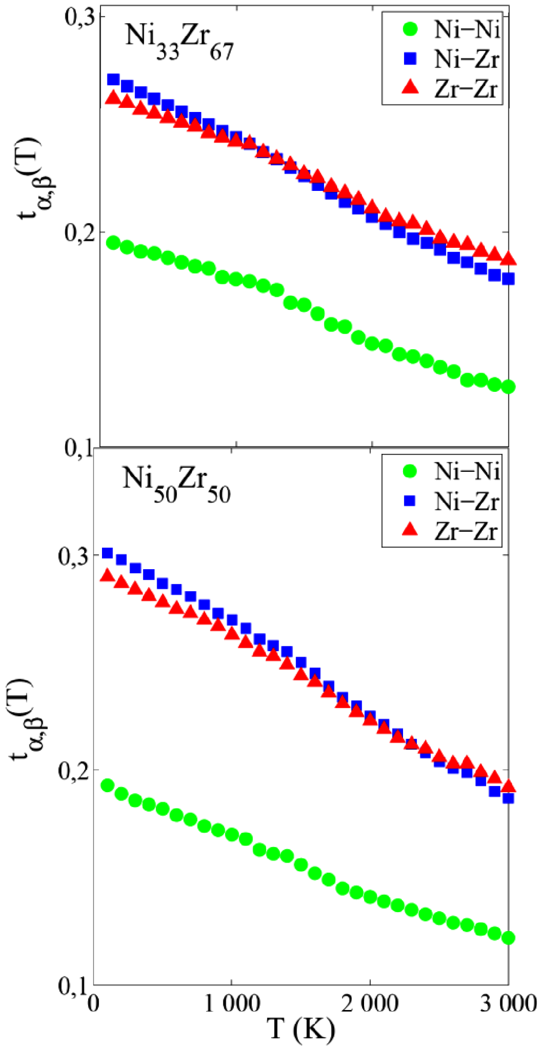

Fig. 2. Translational order parameter for $Ni_{33}Zr_{67}$-system (top panel) and $Ni_{50}Zr_{50}$-system (bottom panel).

$$Q_l = \left(\frac{4\pi}{2l+1} \sum_{m=-l}^{l} \left| \frac{\sum\limits_{i=1}^{N} \sum\limits_{j=1}^{N_b(i)} \Upsilon_l^M(\theta_{ij}, \phi_{ij})}{\sum\limits_{i=1}^{N} N_b(i)} \right|^2 \right). \quad (3)$$

Here, $Y_{lm}(\theta_{ij}, \varphi_{ij})$ are the spherical harmonics, θ_{ij} — the spherical angle, φ_{ij} — the azimuthal angle. N_b is the number of particles neighboring with the i-th particle. At this point under the nearest environment we mean only those particles, which are arranged into the sphere with the radius corresponding to the location of the first minimum in the radial distribution function. For the ideal fcc-structure the value of the parameter q_6 is equal to 0.5745. The numerical values of the parameter $q_6$for the systems $\mathrm{Ni_{33}Zr_{67}}$ and $\mathrm{Ni_{50}Zr_{50}}$ at the temperature $T = 100$ K are presented in Table II.

TABLE II

The orientational order parameter q_6.

$\mathrm{Ni_{33}Zr_{67}}$		$\mathrm{Ni_{50}Zr_{50}}$	
Ni-Ni	0.09924	Ni-Ni	0.00966
Zr-Zr	0.01159	Zr-Zr	0.01912

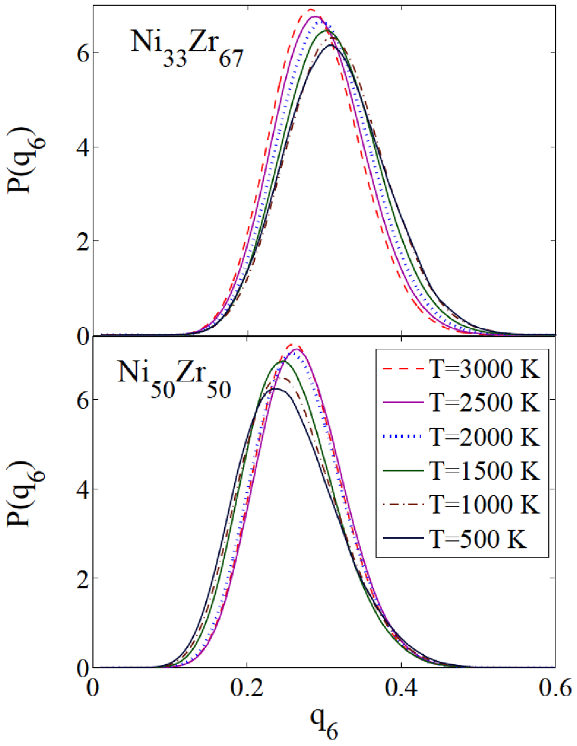

Fig. 3. Probability distribution functions of the local order parameter q_6 for $\mathrm{Ni_{33}Zr_{67}}$-system (top panel) and $\mathrm{Ni_{50}Zr_{50}}$-system (bottom panel).

It can be seen that the values of the orientational order parameter, as well as the translational order parameter for the studied systems take very small magnitudes, indicating that the systems $\mathrm{Ni_{33}Zr_{67}}$ and $\mathrm{Ni_{50}Zr_{50}}$ are in the disordered amorphous states. In Fig. 3, the calculated probability distribution functions of the local order orientational order parameter, $P(q_6)$, for the systems $\mathrm{Ni_{33}Zr_{67}}$ and $\mathrm{Ni_{50}Zr_{50}}$ at the temperatures $T = 500 \div 3000$ K are presented. It can be seen that the $P(q_6)$ distributions for the systems $\mathrm{Ni_{33}Zr_{67}}$ and $\mathrm{Ni_{50}Zr_{50}}$ are symmetric with peak positions at the $q_6^{\max} = 0.28 \div 0.31$ and $q_6^{\max} = 0.24 \div 0.265$, respectively.

This means that the systems $\mathrm{Ni_{33}Zr_{67}}$ and $\mathrm{Ni_{50}Zr_{50}}$ are homogeneous disordered systems in which there are apparently no stable localized ordered structures.

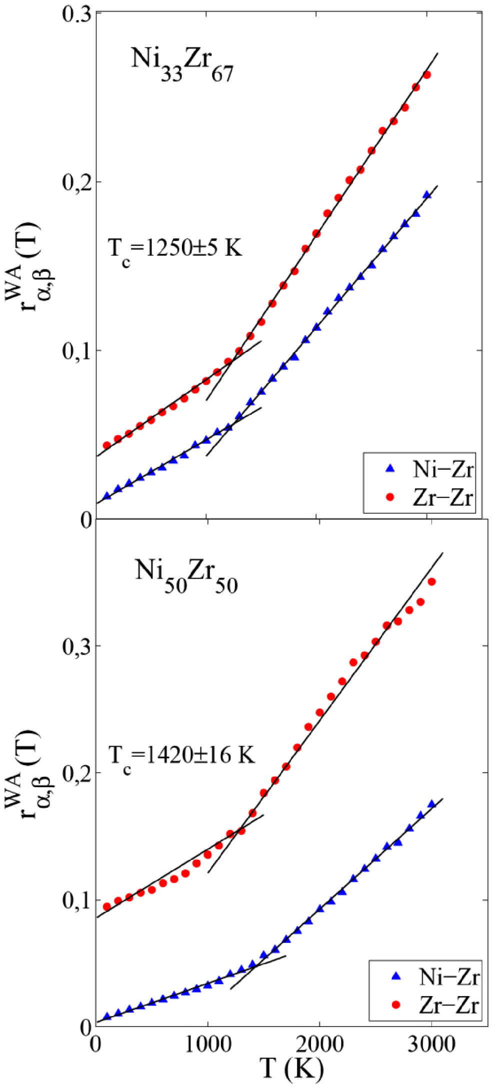

Fig. 3. Wendt–Abraham parameter for $\mathrm{Ni_{33}Zr_{67}}$-system (top panel) and $\mathrm{Ni_{50}Zr_{50}}$-system (bottom panel).

For determination of the glass-forming temperature of the system we have calculated the Wendt–Abraham parameter [11, 12]:

$$r_{\alpha\beta}^{WA} = g_{\alpha\beta}^{\min}(r)/g_{\alpha\beta}^{\max}(r), \quad \alpha, \beta \in \{\mathrm{Ni}, \mathrm{Zr}\}\,. \tag{4}$$

Here, $g_{\alpha\beta}^{\max}(r)$ and $g_{\alpha\beta}^{\min}(r)$ represent the main maximum and the first minimum in the radial distribution function, respectively. Figure 4 shows the temperature dependence of the Wendt–Abraham parameter for various components of the studied system. We have determined the critical glass-forming temperatures for the systems $\mathrm{Ni_{33}Zr_{67}}$ ($T_{\mathrm{c}} = 1250 \pm 5$ K) and $\mathrm{Ni_{50}Zr_{50}}$ ($T_{\mathrm{c}} = 1420 \pm 16$ K) by intersection of the interpolation lines.

4. Conclusion

This work presents the results of computer simulations of molecular dynamics for the metallic systems: $\mathrm{Ni_{33}Zr_{67}}$ and $\mathrm{Ni_{50}Zr_{50}}$. On the basis of the translational and orientational order parameters have shown that in spite of the specific character of the equilibrium distribution functions, the $Ni_{50}Zr_{50}$ system is in the disordered amorphous state. The critical glass-forming temperatures were determined by analysis of the temperature dependence of the Wendt–Abraham parameter. It is shown that increase of the concentration of nickel in the NiZr-system leads to shift of the phase transition point to a higher-temperature region.

References

[1] W. Clement, R.H. Willens, P. Duwez, P. Duwes *Nature* **187**, 869 (1960).

[2] A.L. Greer, *Science* **267**, 1947 (1995).

[3] W.L. Johnson, *MRS Bull.* **24**, 42 (1999).

[4] H. Teichler, M. Guerdane, in: *Phase Transformations in Multicomponent Melts*, Ed. D.M. Herlach, Wiley-VCH, Weinheim 2008.

[5] R.M. Khusnutdinoff, A.V. Mokshin, *Bull. Russ. Acad. Sci. Phys.* **74**, 640 (2010).

[6] R.M. Khusnutdinoff, A.V. Mokshin, I.I. Khadeev, *J. Surf. Invest.* **8**, 84 (2014).

[7] C. Hausleitner, J. Hafner, *Phys. Rev. B* **42**, 5863 (1990).

[8] M.P. Allen, D.J. Tildesley, *Computer Simulation of Liquids*, Clarendon Press, Oxford 1987.

[9] J.R. Errington, P.G. Debenedetti, *Nature* **409**, 318 (2001).

[10] P.J. Steinhardt, D.R. Nelson, M. Ronchetti, *Phys. Rev. B* **28**, 784 (1983).

[11] H.R. Wendt, F.F. Abraham, *Phys. Rev. Lett.* **41**, 1244 (1978).

[12] R.M. Khusnutdinoff, A.V. Mokshin, R.M. Yulmetyev, *JETP* **108**, 417 (2009).