

Elastic properties and glass forming ability of the Zr₅₀Cu₄₀Ag₁₀ metallic alloy

Khusnutdinoff R.M., Mokshin A.V.

Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

Abstract

© 2020 Trans Tech Publications Ltd, Switzerland The elastic properties of the Zr₅₀Cu₄₀Ag₁₀ metallic alloy, such as the bulk modulus B, the shear modulus G, the Young's modulus E and the Poisson's ratio σ , are investigated by molecular dynamics simulation in the temperature range T=250–2000 K and at an external pressure of p=1.0 bar. It is shown that the liquid–glass transition is accompanied by a considerable increase in the shear modulus G and the Young's modulus E (by more than 50%). The temperature dependence of the Poisson's ratio exhibits a sharp fall from typical values for metals of approximately 0.32– 0.33 to low values (close to zero), which are characteristic for brittle bulk metallic glasses. Non-monotonic temperature dependence of the longitudinal and transverse sound velocity near the liquid-glass transition is also observed. The glass forming ability of the alloy is evaluated in terms of the fragility index m. As found, its value is $m \approx 64$ for the Zr₅₀Cu₄₀Ag₁₀ metallic glass, that is in a good agreement with the experimental data for the Zr-Cu-based metallic glasses.

<http://dx.doi.org/10.4028/www.scientific.net/SSP.310.145>

Keywords

Amorphous metallic alloy, Elastic moduli, Glass forming ability, Molecular dynamics, Structural transformations

References

- [1] W.H. Wang, C. Dong, C.H. Shek, Bulk metallic glasses, *Mater. Sci. and Eng.* 44 (2004) 45-89.
- [2] R.M. Khusnutdinoff, A.V. Mokshin, B.A. Klumov, R.E. Ryltsev, N.M. Chtchelkatchev, Structural features and the microscopic dynamics of the three-component Zr₄₇Cu₄₆Al₇ system: equilibrium melt, supercooled melt, and amorphous alloy, *JETP*. 123 (2016) 265-276.
- [3] R.M. Khusnutdinov, A.V. Mokshin, Local structural order and single-particle dynamics in metallic glass, *Bull. Russ. Acad. Sci.: Phys.* 74 (2010) 640-643.
- [4] T. Fujita, P.F. Guan, H.W. Sheng, A. Inoue, T. Sakurai, M.W. Chen, Coupling between chemical and dynamic heterogeneities in a multicomponent bulk metallic glass, *Phys. Rev. B* 81 (2010) 140204(1)-140204(4).
- [5] R.M. Khusnutdinoff, A.V. Mokshin, Electrocrystallization of supercooled water confined by graphene walls, *J. Cryst. Growth*. 524 (2019) 125182(1)-125182(4).
- [6] S. Plimpton, Fast Parallel Algorithms for Short-Range Molecular Dynamics, *J. Comp. Phys.* 117 (1995) 1-19.
- [7] R.M. Khusnutdinoff, A.V. Mokshin, Short-range structural transformations in water at high pressures, *J. Non-Cryst. Solids*. 357 (2011) 1677-1684.
- [8] A.G. Lyapin, E.L. Gromnitskaya, O.F. Yagafarov, O.V. Stal'gorova, V.V. Brazhkin, Elastic properties of crystalline and liquid gallium at high pressures, *JETP*. 107 (2008) 818-827.

- [9] R.M. Khusnutdinoff, A.V. Mokshin, Electrocrystallization of supercooled water confined between graphene layers, *JETP Letters*. 110 (2019) 557-561.
- [10] V.N. Novikov, A.P. Sokolov, Poisson's ratio and the fragility of glass-forming liquids, *Nature*. 431 (2004) 961-963.
- [11] A.V. Mokshin, B.N. Galimzyanov, D.T. Yarullin, Scaling relations for temperature dependences of the surface self-diffusion coefficient in crystallized molecular glasses, *JETP Letters*. 110 (2019) 511-516.
- [12] S.Venkataraman, K. Biswas, B.C. Wei, D.J. Sordelet, J. Eckert, On the fragility of Cu₄₇Ti₃₃Zr₁₁Ni₈Si₁ metallic glass, *J. Phys. D: Appl. Phys.* 39 (2006) 2600-2608.
- [13] S. Pauly, J. Das, N. Mattern, D.H. Kim, J. Eckert, Phase formation and thermal stability in Cu-Zr-Ti(Al) metallic glasses, *Intermetallics*. 17 (2009) 453-462.
- [14] R.M. Khusnutdinov, A.V. Mokshin, R.M. Yulmetyev, Molecular dynamics of liquid lead near its melting point, *JETP*. 108 (2009) 417-427.
- [15] B.N. Galimzyanov, V.I. Ladyanov, A.V. Mokshin, Remarkable nuances of crystallization: from ordinary crystal nucleation to rival mechanisms of crystallite coalescence, *J. Cryst. Growth*. 526 (2019) 125214(1)-125214(4).
- [16] A.V. Mokshin, S.O. Zabegaev, R.M. Khusnutdinoff, Dynamic Heterogeneity of a Colloidal Solution near the Sol-Gel Transition, *Phys. Solid State*. 53 (2011) 570-576.