Dynamic heterogeneities in undercooled metallic alloys: An ab initio molecular dynamics study

N. Jakse

Univ. Grenoble Alpes, CNRS, Grenoble INP, SIMaP, F-38000 Grenoble, France., E–mail: noel.jakse@grenoble-inp.fr

Understanding evolutions of transport properties in undercooled liquids and their interplay with their structural features represents an important issue for solidification processes of metallic alloys, such as crystallization and formation of quasi-crystalline or amorphous phases [1–4]. In the present work, we focus on various classes of Aluminum alloys such as Al-Ni [5], Al-Cu [6], Al-Cr [7] and Al-Zn-Cr [8] that we investigated using ab initio molecular dynamics. We simulate the undercooling process of these alloys during which we monitor the structural and atomic transport properties. We find that diffusion, viscosity and structural relaxation time undergo a crossover between an Arrhenius and non-Arrhenius behavior at a temperature T_X during the slowing down, which corresponds to an onset of dynamic heterogeneities (DHs) that develop. The structural features display characteristics compatible with the occurrence of the icosahedral short-range order (ISRO) as well as the development of a medium range order (MRO) upon cooling. The interplay between the ISRO and MRO and the dynamic heterogeneities is examined. The differences and similarities between these alloys is also discussed.

[1] C. P. Royall and S. R. Williams, Phys. Reports 56, 1 (2015).

[2] H. Tanaka, Eur. Phys. J. E 35, 113 (2012).

[3] Y. Q. Cheng and E. Ma, Prog. Mater. Sci. 56, 379 (2011).

[4] K. F. Kelton, G.W. Lee, A. K. Gangopadhyay, R.W. Hyers, T. J. Rathz, J. R. Rogers, M. B. Robinson, and D. S. Robinson, Phys. Rev. Lett. 90, 195504 (2003).

[5] N. Jakse and A. Pasturel. J. Chem. Phys. 143, 084508 (2015).

[6] N. Jakse and A. Pasturel, AIP Adv. 7, 105212 (2017).

[7] N. Jakse and A. Pasturel, Phys. Rev. B 95, 144210 (2017).

[8] A. Pasturel and N. Jakse, npj Computational Materials 3, 33 (2017).