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Correlations between dynamics and atomic structures in $Cu_{64.5}Zr_{35.5}$ metallic glass[1] C.Z. WANG, Y. ZHANG, F. ZHANG, M.I. MENDELEV, M.J. KRAMER, K.M. HO, Ames Laboratory-USDOE, Iowa State University, Ames, Iowa 50011, USA — The atomic structure of Cu-Zr metallic glasses (MGs) has been widely accepted to be heterogeneous and dominated by icosahedral short range order (ISRO). However, the correlations between dynamics and atomic structures in Cu-Zr MGs remain an enigma. Using molecular dynamics (MD) simulations, we investigated the correlations between dynamics and atomic structures in $Cu_{64.5}Zr_{35.5}$ MG. The atomic structures are characterized using ISRO and the Bergman-type medium range order (BMRO). The simulation and analysis results show that the majority of the mobile atoms are not involved in ISRO or BMRO, indicating that the dynamical heterogeneity has a strong correlation to structural heterogeneity. Moreover, we found that the localized soft vibration modes below 1.0 THz are mostly concentrated on the mobile atoms. The diffusion was studied using the atomic trajectory collected in an extended time interval of 1.2 μs at 700 K in MD simulations. It was found that the long range diffusion in MGs is highly heterogeneous, which is confined to the liquid-like regions and strongly avoids the ISRO and the Bergman-type MRO. All These results clearly demonstrate strong correlations between dynamics (in terms of dynamical heterogeneity and diffusion) and atomic structures in $Cu_{64.5}Zr_{35.5}$ MGs.

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