Fig. S1 :

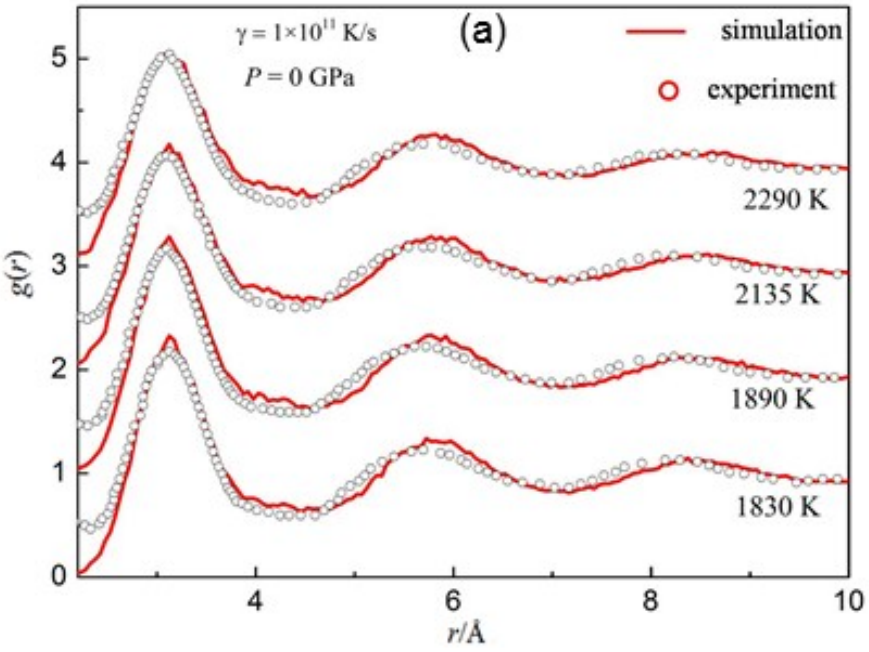

Fig. S1. Comparisons of pair distribution function $g(r)$ between MD simulations and experiments under 0 GPa. The solid lines correspond to the MD simulations, while the open symbols are from the pioneering work by Schenk *et al* [1].

[1] T. Schenk, D. Holland-Moritz, V. Simonet, R. Bellissent, and D. M. Herlach, Icosahedral Short-Range Order in Deeply Undercooled Metallic Melts. *Phys. Rev. Lett*. 2002; **89**: 075507

Fig. S2 :

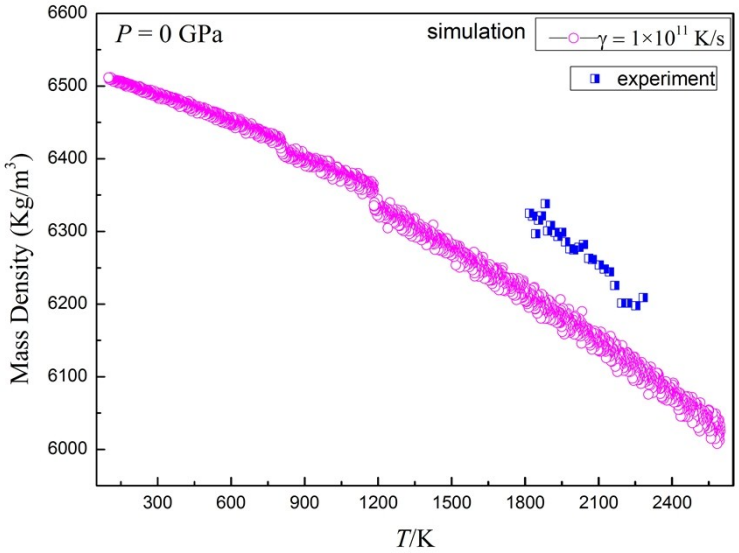

Fig. S2 Comparisons of Mass Density between MD simulation under 0 GPa and experiment [2].

[2] P. F. Paradis and W. K. Rhim, Thermophysical properties of zirconium at high temperature. *J. Mater. Res*. 1999; **14**: 3713

From Fig. S1 and Fig. S2, it can be clearly seen that the simulation are in good agreement with the experiment, which means that the EAM potential function adopted here can reflect the objective physical nature of metal Zr.