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Model inter-atomic potential for Cu-Zr system generated using a multicanonical simulation combined with a first-principles calculation YOSHIHIDE YOSHIMOTO, Department of Applied Mathematics and Physics, Graduate School of Engineering, Tottori University — We can obtain an accurate force field for a molecular dynamics simulation from a first principles calculation. However, the available physical time for a direct first-principles molecular dynamics simulation is often limited to $\sim$ 10 ps because of its high computational cost. If we want to achieve much longer physical time, a possible approach is to build a model inter-atomic potential from a first-principles calculation. As a kind of this approach, Yoshimoto has proposed the "thermodynamic downfolding" method[1,2] which generates an inter-atomic potential based on a multicanonical simulation combined with a first-principles calculation. With this method, we can expect that the thermodynamics of the system is conserved to a maximum extent. In this presentation, application of the method to Cu-Zr system will be reported. This system is interesting because at an composition this system become a bulk metallic glass which has several technologically attracting properties. The melting properties of the system will be covered.

[1] Y. Yoshimoto, J. Chem. Phys., 125, 184103 (2006)
[2] Y. Yoshimoto, J. Phys. Soc. Jpn., 79, 034602 (2010).

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