Probing the self-diffusion process in Aluminium

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Abstract: An in-depth understanding of the diffusion process in liquid metals is a key to design and engineering new high-performance materials. In this study, using molecular dynamics simulations supplemented with the embedded atom potential, we investigate/compare the self-diffusion process in liquid Aluminium. To understand the self-diffusion process, we analyze the radial distribution functions, velocity distributions, mean square displacements, and self-diffusion coefficients at various temperatures well above the melting temperature of Aluminium in the temperature range of 1000 K to 1800 K. As a key result, in both the αα and ββ phases, the self-diffusion coefficients show a non-linear variation with rise in temperatures in the range of 1000 K to 1200 K. From 1300 K to 1800 K, the self-diffusion coefficients increase more or less monotonically with rise in temperature. We found that a higher temperature in the range of 1300 K to 1800 K leads to a greater self-diffusion coefficient, suggesting the more violent movement of the atoms around their equilibrium positions. The results presented in this work can help to understand the differences in the self-diffusion process in the technologically relevant Al phases.