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Molecular Dynamics Analysis on the Dynamic Contact Angle Based on the Extraction of the Stress Distribution in Steady-State Non-Equilibrium Systems of a Single Lennard-Jones Fluid between Solid Walls under Shear HIROKI KUSUDO, TAKESHI OMORI, YASUTAKA YAMAGUCHI, Department of Mechanical Engineering, Osaka University — The Method of Plane (MoP) is a technique to calculate the stress distributions for systems in equilibrium molecular dynamics (EMD) simulations. In this study, we propose a method to extend the MoP to steady-state nonequilibrium molecular dynamics (NEMD) systems based on the velocity distribution function. Moreover, we examined the momentum balance exerted on a control volume set around the contact line for a single fluid between parallel walls under steady shear. By extending Bakkers equation, which connects the stress distribution and solid-related interfacial tension, we showed that the force balance among the dynamic interfacial tensions around the contact line can be rewritten by a model equation equivalent to Youngs equation for equilibrium systems. We applied the model equation for steady state NEMD systems of single Lennard-Jones fluid by calculating the stress distribution, and showed that for the present system, the dynamic solid-liquid interfacial tension was constant sufficiently away from the contact line, and the constant value was almost equal to the static value irrespective of the shear rate tested. This result indicated that the dynamic apparent contact angle was not significantly different from the equilibrium apparent contact angle for the present system.

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