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Synchronized Molecular-Dynamics simulation for thermal lubrication of a polymeric liquid between parallel plates[1] SHUGO YASUDA, University of Hyogo, RYOICHI YAMAMOTO, University of Kyoto — The Synchronized Molecular-Dynamics simulation which was recently proposed by authors [Phys. Rev. X **4**, 041011 (2014)] is applied to the analysis of polymer lubrication between parallel plates. In the SMD method, the MD simulations are assigned to small fluid elements to calculate the local stresses and temperatures and are synchronized at certain time intervals to satisfy the macroscopic heat- and momentum-transport equations.The rheological properties and conformation of the polymer chains coupled with local viscous heating are investigated with a non-dimensional parameter, the Nahme-Griffith number, which is defined as the ratio of the viscous heating to the thermal conduction at the characteristic temperature required to sufficiently change the viscosity. The present simulation demonstrates that strong shear thinning and a transitional behavior of the conformation of the polymer chains are exhibited with a rapid temperature rise when the Nahme-Griffith number exceeds unity.The results also clarify that the reentrant transition of the linear stress-optical relation occurs for large shear stresses due to the coupling of the conformation of polymer chains with heat generation under shear flows.

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