A model of friction through dynamical formation and rupture of molecular bonds
and its extension to the flexible surfaces.

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Abstract

A model for friction in a system of two rigid plates connected by bonds (springs) and experiencing an external drive is discussed. The macroscopic frictional properties of the system are shown to be directly related to the rupture and formation dynamics of the bond subsystem.

Different regimes of motion are characterized by different rates of rupture and formation relative to the driving velocity. In particular, the stick-slip regime is shown to correspond to a cooperative rupture of the bonds. Moreover, the motion of static friction is shown to be dependent on the experimental conditions and time scales. The overall behavior can be described in terms of two Deborah numbers, \( D_1 = \frac{V}{V_c} \) and \( D_2 = \frac{V}{V_0} \), which describe a competition between the rates of bond rupture and formation and the rate of external drive.

However, the model of two rigid plates includes the bonds in a very phenomenological manner. It does not allow one to relate practically the elastic surface transformations with the formation and rupture of the bonds. To go beyond the phenomenology, a model of friction involving two flexible surfaces is proposed. It captures the elastic transformations and molecular exchange between the surfaces. It is based on the solution of coupled microscopic equations partially including the elastic degrees of freedom of the macroscopic (bulk) subsystems. The extended model agrees well with known direct solutions of the friction problems including randomly moving particles in Brownian dynamics or movable cellular automata. It offers a practical approach to investigate response of sheared systems under a broad range of parameters as well as at different time and space scales.