Modeling of nanoindentation of α-graphite using registry-dependent interlayer potential

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Experimental investigations of the nanoscale friction between a tungsten tip of the friction force microscope (FFM) and graphite surface have revealed the existence of superlubricity in such a system. This phenomenon is manifested in a reduction of friction by orders of magnitude. Frictional force in the mentioned system exhibits strong dependence on the scanning direction of the FFM tip with the 60° symmetry of individual atomic layers in the graphite lattice. This fact and the agreement of the experiments with the numerical simulations carried out on the Tomlinson-based model have been the main reasons to argue that the superlubricity took place between the graphite substrate and a graphite flake, attached to the tip. However, in the experiments, there is no firm evidence for the cleavage of the flake and, to our knowledge, the existing theoretical models of superlow friction of graphite are based on the assumption of the presence of a graphene flake.

Here, we offer molecular dynamics simulations which reproduce flake formation for α-graphite. The graphite sample consists of three graphene layers with AB stacking. The bottom layer is static, covalent bonds between atoms in the remaining two dynamic layers are described via Brenner potential. For interlayer interactions registry-dependent potential with local normals by Kolmogorov is used. It is designed in such a manner that long-ranged van der Waals as well as short-ranged orbital overlap contributions to the cohesion in layered graphitic structures are taken into account. The sample is indented with adhesive absolutely rigid pyramidal tip and the heat is dissipated via Berendsen thermostat applied to all dynamic atoms. The influence of the value of interactions between carbon and tip atoms, the distance between atoms in the tip and the rate of indentation on the behaviour of the system are examined. The obtained force-versus-distance curves resemble experimental ones with jump-to-contact during loading phase and hysteresis during unloading. It is shown that flake formation takes place for higher values of carbon-tip interactions and indentation rates.