Atomistic simulation of the tribological properties of Cu and Au nanoparticles adsorbed on a graphene sheet

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This work has a goal to study the behavior of metal nanoparticles (NP) on the graphene layer. Using classical molecular dynamics method we have accomplished three series of computer experiments. Objects of study were Au and Cu NP. Sizes of particles are between 10 and 30 thousands atoms. Vacuum conditions were maintained. Atoms on the edges of layer were fixed. Also periodic boundary conditions were used. Embedded atom method was used to simulate interaction between metal atoms. Harmonic potential was used for modeling carbon atoms behavior. Interaction between metal and carbon atoms is based on Lennard-Jones potential. The process of modeling itself can be divided into two parts: 1) obtaining a NP; 2) shear of NP. In the first part the layer of metal atoms is placed onto the graphene layer. Interaction energy between atoms of metal is stronger than between metal and carbon atoms. The metal layer starts to fold into NP. At this time energy is released, the temperature of system is growing. At some point we use Berendsen thermostat to cool nanoparticle and graphene layer. The second part is the most informative one. After NP is formed, it is sheared. Shear force is applied to all atoms located on the left side to center of mass of NP. The force grows until the velocity of NP is 3.55 m/s. After that shear force remains constant, NP is moving with constant acceleration.

During the experiment different system parameters are measured: potential energy, temperature, size of NP, friction and shear forces, velocity of center of mass of NP. After processing obtained data we have studied dependence between friction force and contact area of NP, in all cases it is linear. This conclusion is confirmed by real experiment results. Dependence between friction force and lateral coordinate of center of mass has a sawtooth form. After three series of experiments we can say that dependence between friction force and temperature takes place. On the growth of temperature the friction force is decreasing for Cu and Au NP. However the dependence is complicated, more research has to be done.