Nanodroplet impact onto solid platinum surface: Spreading and bouncing

DANIEL LUSSIER, YIANNIS VENTIKOS, Dept. Engineering Science, Univ. of Oxford — The impact of droplets onto solid surfaces is found in a huge variety of natural and technological applications, from rain drops splashing on the pavement, to material manufacturing by molten droplet deposition. Taking inspiration from existing microfluidic technologies (i.e. lab-on-chip), there is increasing interest in the use of nanodroplets (D < 100 nm) for a number of applications such as drug delivery and semiconductor device manufacturing. However, as the size of the droplet is reduced into the nanoscale, the direct use of previously obtained macroscopic results is not guaranteed. At the nanoscale, important effects due to the molecular nature of the fluid, thermal fluctuations and reduced dimensionality can play a critical role in determining system dynamics. In this paper we present the results of large-scale, fully atomistic, three-dimensional molecular dynamics (MD) simulation of an argon nanodroplet (D = 18 nm, 54 000 atoms) impact onto a solid platinum surface, using the LAMMPS software package. The fluid argon is modeled using the well-known Lennard-Jones (LJ) potential, while the embedded-atom model (EAM) potential is used for the solid platinum. By varying both the impact velocities (10-1000 m/s) and the wettability of the solid surface a wide range of impact behaviors is observed, from smooth spreading, to bouncing recoil, pointing towards a wide array of potential applications.

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