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NICS

Theoretical Studies of the De-wetting Mechanism of Metallic Thin-Films

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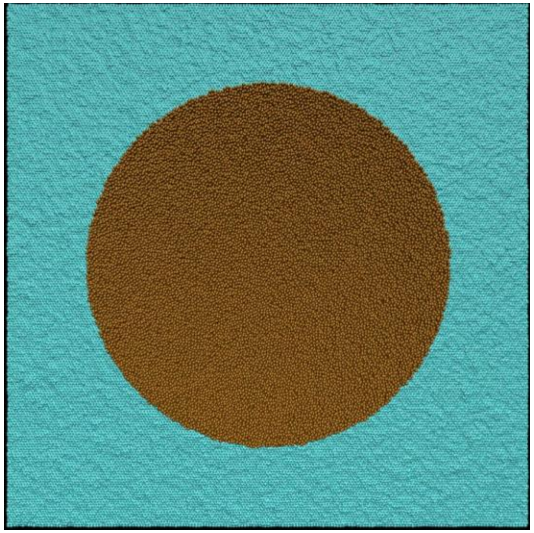
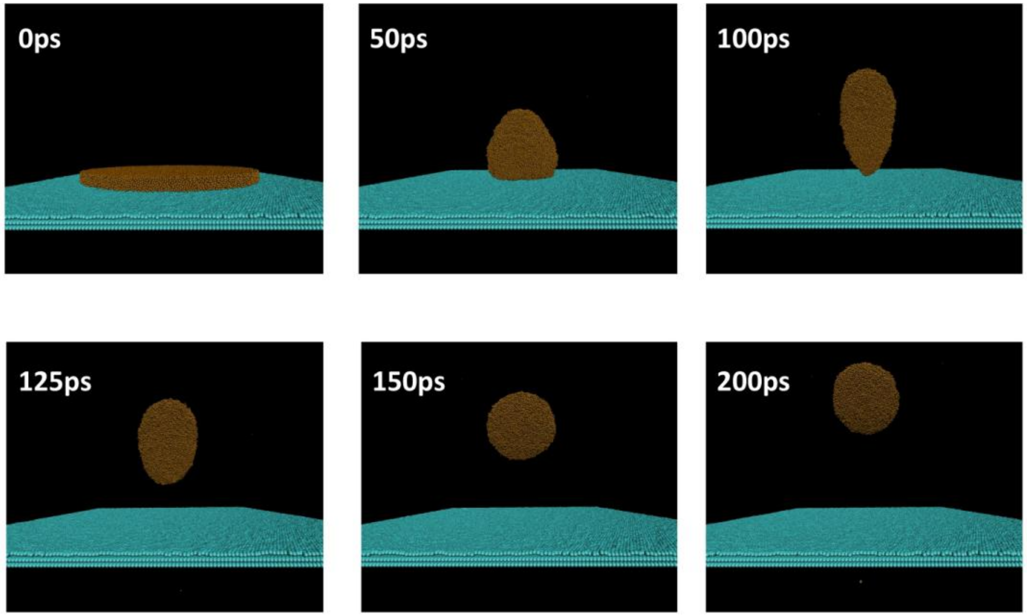
Project scope

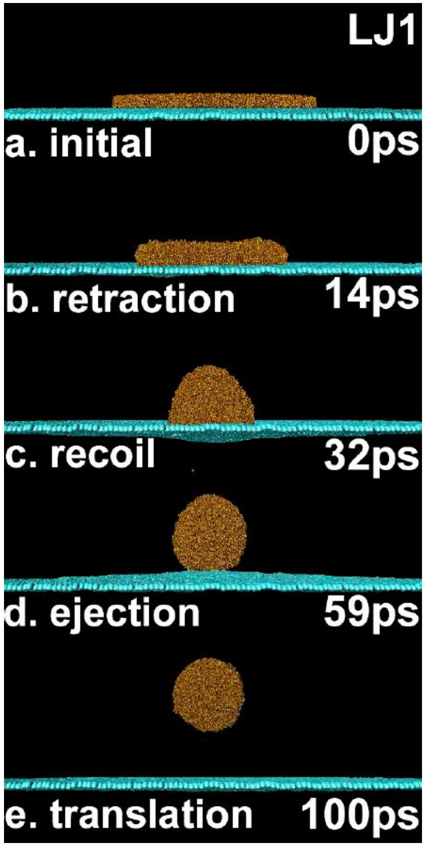
- Thin film de-wetting can be exploited to self-assemble and organize nanoparticles. To control self-assembly and organization, it is crucial to understand the nanoscale liquid phase dynamics. In this respect, Molecular Dynamics simulations (MD) using a Lennard-Jones (LJ) potential is a powerful tool.
- We used different LJ potentials to investigate the de-wetting of a Cu liquid circle at a temperature, T, of 2200 K on graphiten (see below). The simulations were performed with the software LAMMPS, which is installed in Kraken. The systems, which consisted of about 300,000 atoms, were simulated for 200ps in about 1,000 processors at most.



De-wetting mechanism

- **When the potential is very weak, the circle jumps off the graphitic substrate with a velocity of the order of 100 m/s [1] (below, left). (This result mimics very well previous experimental results for Au triangles on graphite/silica.) This finding let us to consider a nanotrampoline-like configuration in which a liquid Cu-circle de-wets when placed on top of a graphene membrane (below, right) [1].**

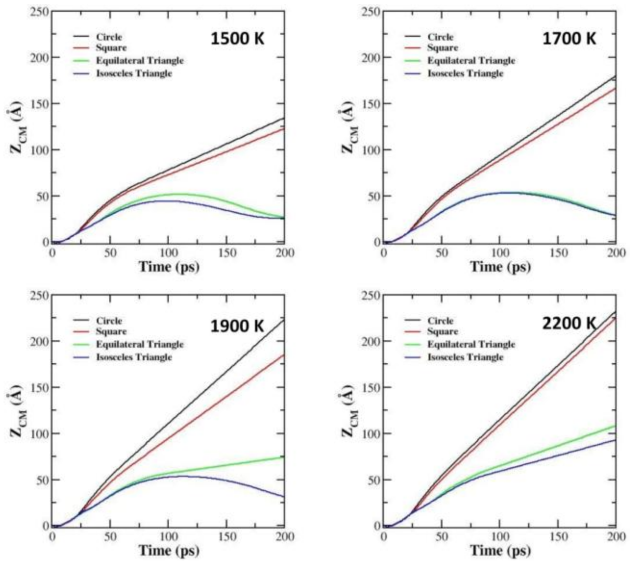


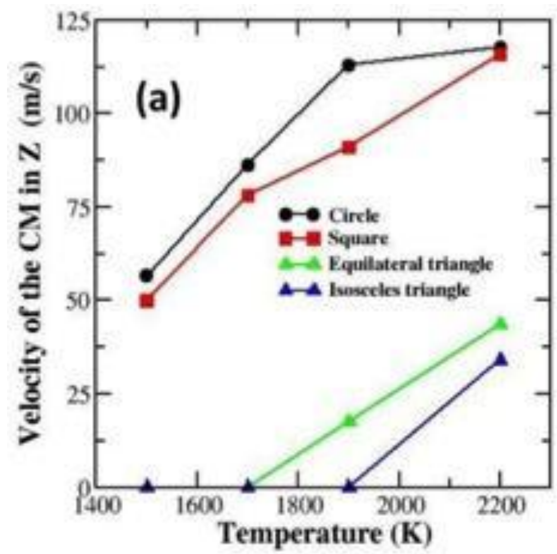


[1] Fuentes-Cabrera, M.; Rhodes, B. H.; Fowlkes, J. D.; Lopez-Benzanilla, A.; Terrones, H.; Simpson, M. L.; Rack, P. D., *Phys Rev E* 2011, *83*, 041603.

Investigating the jumping velocity

- **The previous theoretical results, and our previous experimental knowledge that different initial shapes lead to different de-wetted structures, led us to investigate whether the jumping velocity could be modified via the initial shape and temperature**



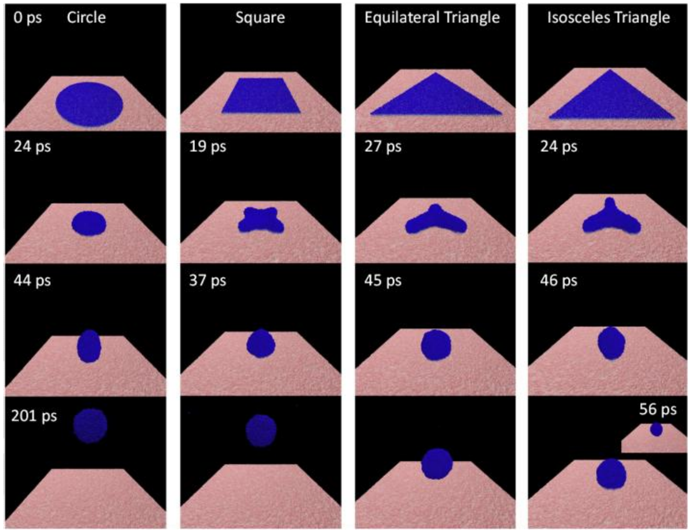


As seen above, the more symmetric is a nano-structure, the faster it jumps. Similarly, the higher is the initial T, the faster a nano-structure jumps [2].

[5] Miguel Fuentes-Cabrera, Bradley H. Rhodes, Michael I. Baskes, Humberto Terrones, Jason D. Fowlkes, Michael L. Simpson and Philip D. Rack. ACS Nano, DOI: 10.1021/nn2018254

Further analysis

- Further analysis, see above, revealed that the dependence of the ejected velocity on shape is ascribed to the temporal asymmetry of the mass coalescence during the droplet formation. The dependence on temperature, on the other hand, is ascribed to changes in the density and viscosity.



Our results suggest that de-wetting induced by nanosecond laser pulses could be used to control the velocity of ejected nanodroplets, which opens up a new realm of possibilities towards the control and guidance of nanoscale objects [2].

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