

Abstract Submitted
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Continuum Models of Nanoscale Effects in Initial Stages of Droplet Coalescence and Wetting MYKYTA V. CHUBYNSKY, Mathematics Institute, University of Warwick, UK, SREEHARI PERUMANATH, School of Engineering, University of Edinburgh, UK, SALAH KOUHEN, Mathematics Institute, University of Warwick, UK, ROHIT PILLAI, School of Engineering, University of Edinburgh, UK, JAMES E. SPRITTLES, Mathematics Institute, University of Warwick, UK, MATTHEW K. BORG, School of Engineering, University of Edinburgh, UK — In molecular dynamics (MD) simulations of nanodrop coalescence [1] and wetting two non-classical effects are observed. First, despite the axial symmetry of the problems of impact and head-on drop-drop collisions, initial contact generally occurs away from the symmetry axis due to thermal fluctuations of the droplet surface. Second, in initial stages of coalescence/wetting, growth of the liquid bridge/contact area mostly occurs via transverse jumps of the liquid molecules across the gap, rather than via lateral motion expected classically. For the first effect, we consider stochastic differential equations for the modes of surface deformation to obtain results for the distribution of contact points, in good agreement with MD. For the second effect, we solve numerically Navier-Stokes equations with a disjoining pressure derived from the Lennard-Jones potential used in MD and thus having both an attractive and a repulsive term. Attraction causes the droplet surface to accelerate towards the surface it is coming in contact with and reach a significant speed by the time of contact, which contributes to the motion of the contact line, as in MD. [1] S. Perumanath *et al.*, Phys. Rev. Lett. 122 (2019) 104501.

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