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Homogeneous nucleation of Lennard-Jones liquids HUI WANG, HARVEY GOULD, Clark University, W. KLEIN, Boston University — We investigate the homogeneous nucleation of a Lennard-Jones liquid as a function of the degree of supercooling. The umbrella sampling method, with the size of the largest cluster as the order parameter, is used to compute the free energy cost of the nucleating droplets. Their saddle point nature is verified using an intervention technique. For moderate supercooling the nucleating droplets are found to be compact and spherical, with the core having fcc symmetry and the surface bcc. As the system is quenched near the spinodal, which corresponds to the vanishing of the free energy barrier, the nucleating droplets become more diffuse and anisotropic with no well defined core or surface. The environment of these nucleating droplets form randomly stacked planes, which is consistent with the spinodal nucleation picture.

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