MD SIMULATIONS OF FRICTION AND WEAR OF FUEL SURROGATES

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Fig.1 This is a snapshot of a molecular dynamics simulation system. In this system, a 50:50 mixture of toluene (blue molecules) and butylcyclohexane (red molecules) are confined between two ultrananocrystalline, UNCD, coatings (gray spheres). Hydrogen atoms on the confined fuel molecules are not shown for clarity. The outer red and blue UNCD layers are thermostated and held rigid, respectively. The distance between the rigid layers is changed to control the load and the upper surface is slid to the right to simulate sliding.

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