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Molecular Dynamics investigation into the mechanism of damage of Ni-Ni trobopair system during high-velocity sliding

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ABSTRACT This paper investigated the mechanisms of subsurface damage and material removal of sliding blocks under nanoscale high velocity friction. The analysis was carried out with the aid of three-dimensional molecular dynamics simulation. The process of structure changing was observed and the number of different types of atoms was analyzed, which is help to find out the mechanism of damage. The microstructure of both the sliding block and the stationary block are observed to study the changing of frictional characteristic. Several snapshots of the deformation zone at different time and different velocity are shown to investigate the effect of the sliding velocity on sliding. The result shows that the damage region develops through three stages. The hexagonal close-packed（HCP） structure is a transition during damage. Higher sliding velocity results in more damage and lower inner pressure in the sliding block. interfaces between the amorphous portions and Face Centered Cubic（FCC ）portions have bigger temperature gradient and larger heat flux.

Keywords: molecular dynamics, damage, structure, high velocity