

Abstract Submitted  
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**Large Scale Atomistic Modeling of Scratching Process by a Spherical Tool**<sup>1</sup> BEHROUZ SHIARI, University of Michigan — Large molecular dynamics simulations are performed to investigate the nanoscale scratching process of monocrystalline nickel. The effects of scratching velocities and temperature of the substrate on the resulting chip formation, scratching forces, dislocation nucleation and propagation, and finally workpiece surface evolution are studied. The results show that the scratching resistance increases with the increase in scratching velocity. The higher scratching velocity results in larger chip volume and closer chip shape with a more amorphous structure. Simulations also show that the scratching force fluctuations can be correlated to nucleation and propagation of dislocations in the substrate. The dislocations nucleated during scratching dissociate into Shockley partial dislocations connected with a band of stacking fault as they propagate along a V-shape pattern. These patterns can be observed as hillock marks on the scratching free surface a short distance from the tool position. The fluctuation of scratching force is affected by the scratching velocity and the drops and rises of the scratching forces disappear at high scratching velocities due to high strain rate. The atomic scale behavior changes with temperature, and the clear drops and rises of the scratching force can not be observed at higher temperatures.

<sup>1</sup>The use of NNIN computation resources at the University of Michigan is appreciated.

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