Atomistic Insights on the Wear/Friction Behavior of Nanocrystalline Ferrite During Nanoscratching as Revealed by Molecular Dynamics


Abstract:

Using embedded atom method potential, extensive large scale molecular dynamics (MD) simulations of nanoindentation/nanoscratching of nanocrystalline (nc) iron have been carried out to explore grain size dependence of wear response. MD results show no clear dependence of the frictional and normal forces on the grain size; and the single crystal (sc) iron has higher frictional and normal force compared to nc-samples. For all samples, the dislocation mediated mechanism is the primary cause of plastic deformation in both nanoindentation/nanoscratch. However, secondary cooperative mechanisms are varied significantly according to grain size. Pileup formation was observed in the front of and sideways of the tool, and they exhibit strong dependence on grain orientation rather than grain size. Tip size has significant impact on nanoscratch characteristic, both frictional and normal forces monotonically increase as tip radii increase while the friction coefficient value drops by about 38%. Additionally, the increase of scratch depth leads to an increase of frictional and normal forces as well as friction coefficient. To elucidate the relevance of indentation/scratch results with mechanical properties, uniaxial tensile test was performed for nc-samples, and the result indicate the existence of both the regular and inverse Hall-Petch relations at critical grain size of 11.09 nm. The present results suggest that indentation/scratch hardness has no apparent correlation with the mechanical properties of the substrate whereas the plastic deformation has.

Keywords:

atomistic, polycrystalline iron, scratch hardness, wear, dislocations, twinning.

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