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Formation of tribolayer on sputtered MoS2 and MoSe2 coatings: nanotribology and simulation

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We prepared series of MoS2 and MoSe2 coatings deposited on Si wafers by d.c. magnetron sputtering. The deposition conditions, such as argon pressure, substrate heating, bias, etc., were varied in order to obtain dense films with various microstructures ranging from fully amorphous to highly crystalline films. The coating structure and chemical bonding was identified by transmission electron microscopy (TEM), Raman spectroscopy and X-ray photoelectron spectroscopy. The tribological properties of the coatings were evaluated at various scales: i) by pin-on-disc with alumina ball as a counterpart, and ii) by Friction Force Microscopy (FFM). To evaluate structural changes at sliding interface after the tests produced by macroscopic tribological testing, TEM and Raman spectroscopy were used. As expected, we observed formation of tribolayer consisting of MoS2 or MoSe2 ultra-thin crystal with basal planes oriented in parallel to the surface. In case of FFM, only material transferred onto tip was characterized. Our ambition was to demonstrate that nanoscale FFM can result in similar tribolayer formation observed in macroscopic sliding contact. To understand sliding-induced structural re-ordering of the films with various crystallinity, we present molecular dynamic model of MoS2 sliding process.

Keywords
friction
MoS2
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molecular dynamics