Contribution ID: **160** Type: **Poster Presentation**

Surface Properties of Nickel and Silver Metals

Molecular dynamics (MD) simulation methods were used to study the surface properties of nickel (Ni) and silver (Ag) metals. Calculations were performed at room temperature with the help of DLPOLY computer code. The many-body Sutton-Chen potentials were used to understand the interactions between atoms in both Ni and Ag surface systems. Stability patterns of three basic surfaces {(100), (110) and (111)} of Ni and Ag were determined from the calculated individual surface energies. Radial distribution functions were also extracted for different surface planes. Data extracted from the radial distribution functions suggest that the surface planes studied have solid crystal structures. The (111) surfaces were found to be the most stable for both Ni and Ag metal and the correct stability pattern was confirmed in both metals.

Apply for student award at which level:

None

Consent on use of personal information: Abstract Submission

Yes, I ACCEPT

Primary authors: MATSHABA, Malili (CPhy Membership); Mr MATLALA, Mashilo; Dr MAHLADISA, Mokete; Prof. MOSUANG, Thuto

Presenter: MATSHABA, Malili (CPhy Membership)

Session Classification: Poster Session

Track Classification: Track A - Physics of Condensed Matter and Materials