Research Proposal-1

Study on low-energy Sputtering of Pt atoms impacts on Pt(111)surface: by molecular dynamics simulations

AIMS AND OBJECTIVES

In the presence work we will study the sputtering of pt atoms impacts on pt(111)surface at low temperature in which we will focus.

- Atomic interaction potential of Pt on Pt(111) surface.
- The effect of kinetic energy of Pt incident atom on the substrate at fix temperature.
- The effect of incident energy on the sputtering yield, adatom yield and vacancy yield from the first layer of substrate.
- To calculate diffusion coefficient D, mean square displacements that will be calculated and monitored through out the motion.
- Explanation of diffusion phenomena can be manipulated with the help of movies of the island diffusion.

Research Proposal-2

Hetero-Diffusion of Silver (Ag) Clusters on different surfaces of Copper (Cu)

AIMS AND OBJECTIVES

Attention will be focused on diffusion of Ag Islands (monomer, dimer, trimer, tetramer and up to 10 atoms) on the different low index surfaces of Cu: such as (1 0 0), (1 1 0) and (1 1 1) surfaces. Molecular dynamics technique will provide the trajectory during the process of diffusion of islands. Trajectories of Islands dynamics will be monitored through movies. Diffusion will be carried out at three different temperatures, namely 300, 500 and 700 K.

Mean square displacement will be calculated using all statistics recorded during the diffusion mechanism after each 0.05 ps. Mean square displacement at different time steps will provide rate of diffusion. All this data will be used to deduce diffusion coefficient and excitation energy of the clusters.

Research Proposal-3

Study of dynamics of Au and Ag trimer adatoms on compact surfaces at different temperatures

AIMS AND OBJECTIVES

We will study about the dynamics of Ag and Cu at different temperatures (300 K, 500 K, 700 K) for trimer case.

- Attension will be focus on the diffusion of Cu/Ag(111), Ag/Cu(111) and Ag/Ag(111) in which fissure, dislocation, diffusion coefficient, effective energy barrier and diffusion prefector will be calculated.
- In order to calculate diffusion coefficient D, mean square displacements will be calculated which will be monitored through out the motion.
- During the diffusion of Cu/Ag(111) Ag/Cu(111) and Ag/Ag(111) surfaces vacancies will examined by rising of temperature.
- Arrahanuis law will be used to calculate the effective energy barrier and diffusion prefactor for fcc to hcp and hcp to fcc lattice site hopping.

Research Proposal-4

Estimation of thermal properties of Pd and Pt: A Molecular Dynamics approach

AIMS AND OBJECTIVES

In the present work we will study the thermal properties of Pd and Pt for which lattice parameter, mean square distribution, radial distribution function and energy per atom at various temperatures will be calculated. With the help of these parameters following thermal properties will be estimated

- Thermal Coefficient of linear expansion
- Specific heat
- Melting temperature

Vacancies and twin-boundaries will be generated at specific temperature and effect of defects on above said thermal properties will be estimated.