H(D) → D(H) + Cu(111) Collision System: Molecular Dynamics Study of Surface Temperature Effects

Can D. Vurdu*. Ziya B. Güvenç**

*Kastamonu University, Faculty of Arts and Sciences, Department of Physics,
Kuzeykent TR-37100 Kastamonu Turkey (Tel: +90 366- 215-4923;
e-mail: cvurdu@ kastamonu.edu.tr).
**Çankaya University, Electonic and Communication Engineering Department.,
Yüzüncüyıl Balgat TR-06530 Ankara Turkey (Tel: +90 312-284-4500/130
e-mail: guvenc@cankaya.edu.tr).

Abstract: Reaction dynamics of gas-phase H(or D) atoms with D(or H) atoms adsorbed onto a Cu(111) surface have been studied by micro canonical quasi-classical molecular dynamics simulations. The surface was prepared at different temperature values such as; 30K, 94K and 160K. The adsorbates were distributed randomly on the surface to create 0.18ML, 0.28ML, and 0.50 ML of coverages. The multi layer slab is formed by an embedded-atom many-body potential energy function. The slab atoms can move according to the exerted external forces. Treating the slab atoms non-rigid has a significant effect on the dynamics of the simulation. Significant energy transfer from the projectile atom to the lattice atoms takes place especially during the first impact that modifies significantly the details of the dynamics of the collisions. Therefore effects of different temperatures of the slab are investigated in this study. Interaction between the surface atoms and the adsorbates is modeled by a LEPS function. The LEPS parameters are determined by using the total energy values which were calculated by a density functional theory and generalized gradient approximation for an exchange-correlation energy for many different orientations, and locations of one- and two-hydrogen atoms on the Cu(111) surface. The RMS value of the fitting procedure is about 0.16 eV. Many different channels of the processes on the surface have been examined such as; inelastic reflection of the incident hydrogen, subsurface penetration of the incident projectile and adsorbates, sticking of the incident atom on the surface. In addition, the hot-atom and Eley-Rideal processes are investigated. The hot-atom process is found to be more significant than the Eley-Rideal process. Furthermore, the rate of subsurface penetration is larger than the sticking rate on the surface. In addition, these results are compared and analyzed as a function of the surface temperatures.

Keywords**:** Potential Energy Surface, LEPS, Surface chemistry, Adsorption, Hydrogen