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Knocking on surfaces : interactions of hyperthermal particles with metal surfaces

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Summary

Processes at interfaces are essential for science and technology. They are relevant for the semiconductor industry, the chemical industry, the environment and even for life itself. Therefore, the understanding of such processes is important both in real life and *in silico*. Gas-surface interactions, such as chemical reactions, adsorption and scattering, have been extensively studied because they are prototypical of more complex interactions and make it possible to deepen our knowledge of those processes and to validate advanced computer models. Hence the experiments in this thesis have been carried out under well-defined condition, namely ultrahigh vacuum (UHV). The thesis is primarily focussed on the interaction of hyperthermal particles with Ru(0001) and Ag(111).

Results for scattering of hyperthermal Ar from Ru(0001) and Ru(0001)-(1×1)D are given in **chapter 2** and compared with Ar scattered from Ag(111). We show a dramatic difference in surface topology and stiffness between the Ru and Ag surfaces, despite these elements have similar atomic mass and near-identical surface structure. It is found that hydrogen act to makes the Ru surface even stiffer.

In **chapter 3** the dynamics of hyperthermal Ar interacting with CO-covered Ru(0001) is described. Collision-induced desorption of CO occurs. The absence of immediate CO desorption indicates that the incident Ar cannot readily penetrate the saturated CO overlayer. The dynamics of surface modifications are probed not only by measuring the angle-resolved desorbed CO intensity and energy distributions but also the correlated Ar distributions.

In chapter 2 and 3, Ar is used as the probing and driving atom for hyperthermal particle-surface interaction. Since Ar is an inert atom and the energy used is hyperthermal, the interaction is mainly repulsive in nature. From chapter 4 we progress to studying chemisorption (attractive) interactions. **Chapter 4** deals with the influence of pre-adsorbed CO on the dissociative adsorption of D₂ on Ru(0001). From the experimental results and a simple model, it is found that CO poisons D₂ dissociation not only sterically but also by modifying the locally surface electronic structure up to the nearest-neighbour Ru atoms.

Using N and Ar atoms, chemisorption and physisorption interactions are directly compared in **chapter 5**. Measurements on scattering of hyperthermal N atoms from the Ag(111) surface are presented. The experiments are carried out at a surface temperature of $T_s=500, 600$ and 730 K, above the temperature for recombinative desorption of adsorbed nitrogen. N atoms scattering behaviour is very different from

that of Ar, which is physisorption system. The distribution of scattered N atoms has a very large angular spread and is composed of a broad distribution and a sharp peak. In contrast, the scattered Ar distribution has only a sharp peak. Taking into account the relative masses, N atoms lose energy at the surface more efficiently than Ar atoms. The N results can be explained in terms of a large proportion of the incident N atoms probing a highly corrugated surface due to their interaction with the deep chemisorption potential.

In the final chapter of thesis, **chapter 6**, the interactions of hyperthermal N atoms and N₂ molecules with N-covered Ag(111) held at 300 K is addressed. The results are compared with those from the clean surface at 500 K. The angular intensity and energy distributions of both scattered N and N₂ are similar to those from bare Ag(111). N₂ shows a sharp angular intensity distribution, and its energy loss is very small for both surfaces. However, additional N₂ intensity at small outgoing angles is evident only from the N-covered surface. The possible origins of this N₂ component around the normal are discussed in terms of backscattering and a direct abstraction reaction.