Classical Molecular Dynamic Simulation of Gold Cluster Deposition on TiN (001) Surface.

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Abstract

Metal deposition constitutes one of the most appealing methods for the preparation of new materials of technological interest (catalysis, gas sensors,…). Addition of metal atoms to a surface can in principle look for different targets. Thus, a given relatively inert surface can be promoted by adding an alkali metal like Na. In another direction, specific catalysts are prepared by supporting transition metal atoms on inert surfaces. In a particular case, gold particles supported on surface oxide have been reported to be highly active especially at room temperature. In order to study such phenomenon several questions are relevant from a microscopic point of view. First we are interested by the properties of the metal surface interface: the nature of the bond, the extension of the surface reduction, etc. Secondly, we would like to know the detailed structure of the particles adsorbed at the surface. This information could help for both a better understanding of the interface and a suitable description of the active sites in a given surface reaction. As inert support we have considered the titanium nitride TiN (001) surface and a gold cluster has been deposited. The interface gold-nitride has been studied in a previous work by deposition of single Au atoms on a 1×1 five-layer-thick in a super-cell model. Such calculation were performed using VASP code in a periodic Density Functional Theory framework by using augmented planes-waves as wave function and 8 special point in the reciprocal space. The generalized gradient approximation (GGA) of Pedew *et al.* was used as density functional. In this work, with the aim of simulating a more real characteristics of the materials, including a big number of atoms, the classical dynamic simulations were done. The interaction potentials Au-Ti, Au-N and Au-Au were obtained from DFT periodic calculation using a new method of separation of the interaction of two films of atoms. The classical simulations involved the simultaneous displacements of more than 1000 atoms including surface and adsorbed gold cluster particle. The classical simulation were performed by using DL_POLY code.