Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Hydrogen Adsorption on Stepped Surfaces of Metal Nickel[1]
HUIQIU DENG, HAIXIA XIAO, WANGYU HU, Department of Applied Physics, Hunan University, Changsha 410082, P. R. China — The chemisorption of gas molecules on transition-metals' surfaces has been an attractive field due to its importance in understanding the mechanisms of catalytic reactions. In the present paper the adsorption of hydrogen on nickel stepped surfaces (210), (211), (311), (410), (511), (977) and the low-index surfaces are studied with the embedded-atom model (EAM) many-body potentials which are based on density functional theory. The stable adsorption sites of hydrogen atoms are determined by the adsorption energies. The calculated results show that there exist more active adsorption sites near the steps. It is found that the stepped surfaces affect the adsorption properties of hydrogen seriously. The dissociative adsorption pathways of hydrogen molecules on the different nickel surfaces are also investigated. The results calculated in the present paper are in good agreement with the available experiment data and other theoretical values.

[1]This work is financially supported by the National Natural Science Foundation of China under contract No. 20403004

Huiqiu Deng
Department of Applied Physics, Hunan University
Changsha 410082, P. R. China

Date submitted: 28 Nov 2004 Electronic form version 1.4