Carbide induced reconstruction of monatomic steps on Ni(111) - A density functional study

We present density functional calculations for carbon adsorption at the two types of monatomic steps on a Ni(111) surface. We show that it is thermodynamically favourable to make a carbon induced clock-type reconstruction at the close-packed step with a [111] step geometry, which creates fourfold sites at the step-edge. It is furthermore possible to extend the carbide with the clock reconstructed geometry onto the upper terrace with a net energy gain compared to adsorption of carbon on unreconstructed close-packed steps or terrace sites on Ni(111). Our findings explain the fact that carbide islands start to grow preferentially on the close-packed steps as has been observed using scanning tunneling microscopy.

General information
Publication status: Published
Organisations: Department of Physics, Center for Nanoteknologi
Contributors: Andersson, M., Abild-Pedersen, F.
Pages: 649-655
Publication date: 2007
Peer-reviewed: Yes

Publication information
Journal: Surface Science
Volume: 601
Issue number: 3
ISSN (Print): 0039-6028
Ratings:
Scopus rating (2007): SJR 1.134 SNIP 0.857
Web of Science (2007): Indexed yes
Original language: English
DOIs:
10.1016/j.susc.2006.10.036
Source: orbit
Source ID: 209834
Research output: Contribution to journal › Journal article – Annual report year: 2007 › Research › peer-review