First-principles investigations of Ni3Al(111) and NiAl(110) surfaces at metal dusting conditions

We investigate the structure and surface composition of the γ'-Ni3Al(111) and β-NiAl(110) alloy surfaces at conditions relevant for metal dusting corrosion related to catalytic steam reforming of natural gas. In regular service as protective coatings, nickel–aluminum alloys are protected by an oxide scale, but in case of oxide scale spallation, the alloy surface may be directly exposed to the reactive gas environment and vulnerable to metal dusting. By means of density functional theory and thermochemical calculations for both the Ni3Al and NiAl surfaces, the conditions under which CO and OH adsorption is to be expected and under which it is inhibited, are mapped out. Because CO and OH are regarded as precursors for nucleating graphite or oxide on the surfaces, phase diagrams for the surfaces provide a simple description of their stability. Specifically, this study shows how the CO and OH coverages depend on the steam to carbon ratio (S/C) in the gas and thereby provide a ranking of the carbon limits on the different surface phases.

General information
State: Published
Organisations: Department of Physics, Theoretical Atomic-scale Physics, Haldor Topsoe AS
Pages: 582-592
Publication date: 2011
Peer-reviewed: Yes

Publication Information
Journal: Surface Science
Volume: 605
Issue number: 5-6
ISSN (Print): 0039-6028
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 1.87 SJR 0.81 SNIP 0.759
Web of Science (2017): Impact factor 1.997
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.85 SJR 0.746 SNIP 0.834
Web of Science (2016): Impact factor 2.062
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 1.85 SJR 0.747 SNIP 0.804
Web of Science (2015): Impact factor 1.931
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 1.81 SJR 0.818 SNIP 0.864
Web of Science (2014): Impact factor 1.925
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 1.72 SJR 0.829 SNIP 0.781
Web of Science (2013): Impact factor 1.87
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 1.91 SJR 1.096 SNIP 0.878
Web of Science (2012): Impact factor 1.838
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 1.88 SJR 1.076 SNIP 0.906
Web of Science (2011): Impact factor 1.994
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Original language: English
Keywords: Carbon, Ni3Al, Ni alloys, Metal dusting, Density functional theory, Steam reforming, NiAl, Oxide scale
DOIs: 10.1016/j.susc.2010.12.023
Source: orbit
Source-ID: 276544
Research output: Research - peer-review ; Journal article – Annual report year: 2011