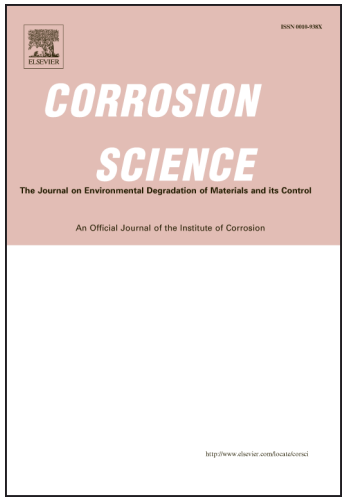

Thermodynamic Assessment of Chemical and Electrochemical Stability of Nickel – Silicon System Alloys

Pavel Anatolyevich Nikolaychuk, Aleksandr Georgievich Tyurin

PII: S0010-938X(13)00133-9
DOI: http://dx.doi.org/10.1016/j.corsci.2013.04.008
Reference: CS 5314

To appear in: *Corrosion Science*

Received Date: 22 June 2012
Accepted Date: 7 April 2013

Please cite this article as: P.A. Nikolaychuk, A.G. Tyurin, Thermodynamic Assessment of Chemical and Electrochemical Stability of Nickel – Silicon System Alloys, *Corrosion Science* (2013), doi: http://dx.doi.org/10.1016/j.corsci.2013.04.008

THERMODYNAMIC ASSESSMENT OF CHEMICAL AND ELECTROCHEMICAL STABILITY OF NICKEL – SILICON SYSTEM ALLOYS

Pavel Anatolyevich Nikolaychuk and Aleksandr Georgievich Tyurin
Chelyabinsk State University, Brat'ev Kashirinykh Street, 129, Chelyabinsk, Russian Federation.
E-mail: npa@csu.ru, tag@csu.ru

Abstract:

Phase and chemical euqilibria in Ni – Si system at 298 K are considered. The possible maximum solid solubility of Si in fcc-Ni at 298 K is estimated.

The Ni – Si – O state diagram at 298 K is plotted. The Ni – Si – O system invariant conditions are calculated. The potential – pH diagram of the Ni – Si – H_2O system at 298 K, air pressure of 1 bar and activities of ions in solution, equal to 1 mol/l is plotted. Basic chemical and electrochemical equilibria in Ni – Si – H_2O system are considered.

Keywords:
A. Alloy;
B. electrochemical calculation;
B. modelling studies;
C. oxidation;
C. Pourbaix diagram;
C. thermodynamic diagrams.

1. Introduction.

In recent years there is growing evidence, indicating the perspectives of using transition metals silicides as new corrosion-resistant materials and coatings. There is currently no systematic studies of their corrosion-electrochemical behaviour, the available data are fragmentary and do not cover all the variety of compounds and corrosion-active environments. There is no single theory that can explain the chemical resistance to corrosion of the existing materials and predict such properties for the new ones [1]. One of the methods to describe the oxidation of silicides both in oxygen-containing gaseous environments (chemical stability) and in water environments (electrochemical stability) is the thermodynamic modelling.

Nickel – silicon is an important binary system, and it has been modelled many times. Moreover, many ternary systems, containing these two elements, such as C – Ni – Si [2], Mo – Ni – Si [3], Ni – Si – V [4], Mn – Ni – Si [5], Ni – Si – O [6], Fe – Ni – Si [7], Cr – Ni – Si [8], Cu – Ni – Si [9], Ni – Si – B [10] and others, are of interest to the researchers. However, almost all published materials correspond to high temperatures. The present study is devoted to thermodynamic description of Ni – Si system at standard temperature only.

2. Phase and chemical equilibria in Ni – Si system at the temperature of 298 K.

According to the Ni – Si phase diagram [11 – 13], several phases exist in system at standard conditions. There are six intermediate phases: β_1 (Ni_3Si), γ (Ni_5Si_2 or $Ni_{31}Si_{12}$ [6]), δ (Ni_2Si), ε (Ni_3Si_2), NiSi and $NiSi_2$. Pure silicon exists in diamond modification, and it seems, that nickel is insoluble in it. At the nickel-rich part of the system, the solid solution of face-centered cubic nickel can be formed. There is no published information about silicon maximum solid solubility at 298 K, but it is relatively high (more that 10 atomic percent) at 1000 K [11].

Although almost all nickel silicides have a narrow homogeneity ranges at 800˚C [13], they can be treated as stoichiometric phases at standard temperature. The standard Gibbs energies of formation of these compounds are summarized in table 1. Values, presented in [6, 10, 13 – 16], are obtained from various CALPHAD assessments of Ni – Si system, while values, presented in [17 – 21], are either experimentally measured or calculated from experimentally measured standard enthalpy of formation and calculated standard entropy of formation from