Modelling Cr depletion under a growing Cr2O3 layer on austenitic stainless steel: the influence of grain boundary diffusion

The oxidation behaviour of austenitic stainless steels in the temperature range 723–1173K is strongly influenced by the grain size of the oxidizing alloy. In this work the evolution of the concentration profiles of Cr, Ni and Fe in the substrate below a growing Cr2O3 layer is simulated with a Fisher-type numerical model, which takes both volume and grain boundary diffusion into consideration. The model is based on a two-dimensional control volume-based solution of Fick's 2nd law for multicomponent diffusion and includes crossterm diffusion coefficients. The oxide layer is assumed to grow according to a parabolic rate law as a consequence of rate limiting diffusion of Cr cations through the oxide layer; the retraction of the oxide/alloy interface associated with the removal of Cr atoms from the substrate is included in the calculations. Numerically, the movement of the oxide/alloy interface is formulated such that the initial mesh can be used throughout the calculation. The calculated concentration profiles of the alloying elements emphasize the importance of grain boundaries in supplying Cr from the alloy to the growing oxide layer. For temperatures of 823 and 923K the simulations predict a significantly lower concentration of Cr atoms in the alloy at the oxide/alloy interface than that predicted by the conventional one-dimensional analytical Wagner solution, where an effective diffusion coefficient at the interface is assumed.

General information
State: Published
Organisations: Department of Mechanical Engineering, Manufacturing Engineering, Materials and Surface Engineering
Pages: 035009
Publication date: 2009
Peer-reviewed: Yes

Publication information
Journal: Modelling & Simulation in Materials Science and Engineering
Volume: 17
Issue number: 3
ISSN (Print): 0965-0393
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 1.8 SJR 0.821 SNIP 0.93
Web of Science (2017): Impact factor 1.793
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 1.82 SJR 1.076 SNIP 1.05
Web of Science (2016): Impact factor 1.891
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 1.73 SJR 1.225 SNIP 1.057
Web of Science (2015): Impact factor 1.859
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 1.81 SJR 1.305 SNIP 1.157
Web of Science (2014): Impact factor 2.167
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 1.25 SJR 1.083 SNIP 1.197
Web of Science (2013): Impact factor 1.492
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 2.05 SJR 1.461 SNIP 1.794
Web of Science (2012): Impact factor 1.932
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 1.96 SJR 1.151 SNIP 1.362
Web of Science (2011): Impact factor 2.298
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.244 SNIP 1.307
Web of Science (2010): Impact factor 1.387
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.16 SNIP 1.165
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.263 SNIP 1.097
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.951 SNIP 1.347
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.045 SNIP 1.416
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.719 SNIP 1.133
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.074 SNIP 1.289
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 0.447 SNIP 0.917
Scopus rating (2002): SJR 0.988 SNIP 1.211
Scopus rating (2001): SJR 1.083 SNIP 1.025
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 0.677 SNIP 0.944
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 0.802 SNIP 0.967
Original language: English
DOIs:
10.1088/0965-0393/17/3/035009
Source: orbit
Source-ID: 241914
Research output: Research - peer-review › Journal article – Annual report year: 2009