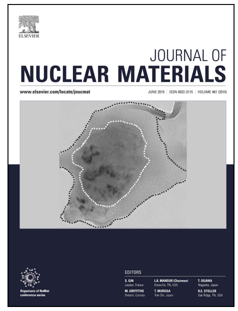
Accepted Manuscript



Atomistic study of the hardening of ferritic iron by Ni-Cr decorated dislocation loops

G. Bonny, A. Bakaev, D. Terentyev, E. Zhurkin, M. Posselt

PII: S0022-3115(17)30583-4

DOI: 10.1016/j.jnucmat.2017.11.016

Reference: NUMA 50625

To appear in: *Journal of Nuclear Materials*

Received Date: 18 April 2017

Revised Date: 26 October 2017

Accepted Date: 10 November 2017

Please cite this article as: G. Bonny, A. Bakaev, D. Terentyev, E. Zhurkin, M. Posselt, Atomistic study of the hardening of ferritic iron by Ni-Cr decorated dislocation loops, *Journal of Nuclear Materials* (2017), doi: 10.1016/j.jnucmat.2017.11.016.

Atomistic study of the hardening of ferritic iron by Ni-Cr decorated dislocation loops

G. Bonny[1], A. Bakaev[1], D. Terentyev[1]*, E. Zhurkin[2], M. Posselt[3]

[1] SCK•CEN, Nuclear Materials Science Institute, Boeretang 200, B-2400 Mol, Belgium
[2] Department of Experimental Nuclear Physics K-89, Faculty of Physics and Mechanics, St.Petersburg State Polytechnical University, 29 Polytekhnicheskaya str., 195251, St.Petersburg, Russia
[3] Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstraße 400, 01328 Dresden, Germany

Abstract

The exact nature of the radiation defects causing hardening in reactor structural steels consists of several components that are not yet clearly determined. While generally, the hardening is attributed to dislocation loops, voids and secondary phases (radiation-induced precipitates), recent advanced experimental and computational studies point to the importance of solute-rich clusters (SRC). Depending on the exact composition of the steel, SRCs may contain Mn, Ni and Cu (e.g. in reactor pressure vessel steels) or Ni, Cr, Si, Mn (e.g. in high-chromium steels for generation IV and fusion applications). One of the hypotheses currently implied to explain their formation is the process of radiation-induced diffusion and segregation of these elements to small dislocation loops (heterogeneous nucleation), so that the distinction between SRCs and loops becomes somewhat blurred. In this work, we perform an atomistic study to investigate the enrichment of loops by Ni and Cr solutes and their interaction with an edge dislocation. The dislocation loops decorated with Ni and Cr solutes are obtained by Monte Carlo simulations, while the effect of solute segregation on the loop's strength and interaction mechanism is then addressed by large scale molecular dynamics simulations. The synergy of the Cr-Ni interaction and their competition to occupy positions in the dislocation loop core are specifically clarified.

PACS : 61.80.Az, 61.82.Bg
Keywords: Iron; ferritic steel; precipitation; dislocation; molecular dynamics

*Author for correspondence. Email: dterenty@sckcen.be, Tel.: +32-14-333197; fax: +32-14-321216