Molecular Dynamics simulation of dislocations in uranium dioxide

Paul Fossati, Laurent Van Brutzel, Benoît Devincre

PII: S0022-3115(13)00947-1
DOI: http://dx.doi.org/10.1016/j.jnucmat.2013.07.059
Reference: NUMA 47651

To appear in: *Journal of Nuclear Materials*

Received Date: 28 April 2013
Accepted Date: 28 July 2013

Please cite this article as: P. Fossati, L.V. Brutzel, B. Devincre, Molecular Dynamics simulation of dislocations in uranium dioxide, *Journal of Nuclear Materials* (2013), doi: http://dx.doi.org/10.1016/j.jnucmat.2013.07.059

Molecular Dynamics simulation of dislocations in uranium dioxide

Paul Fossati[a], Laurent Van Brutzel[a,*], Benoît Devincre[b]

[a] *CEA, DEN, DPC, SCCME, F-91191 Gif-sur-Yvette Cedex, France*
[b] *LEM, CNRS-ONERA, 29 avenue de la Division Leclerc, F-92322 Châtillon Cedex, France*

Abstract

The plasticity of the fluorite structure in UO_2 is investigated with molecular dynamics simulation and empirical potential. The stacking fault energies and the dislocation core structures with Burgers vector $a/2\langle 1\,1\,0\rangle$ are systematically calculated. All dislocation core structures show a significant increase of the oxygen sub-lattice disorder at temperatures higher than 1500 K. The threshold stress for dislocation glide is found to decrease with increasing temperature but its values is always very high, several GPa at 0 K and several hundred of MPa at 2000 K. A relation between the dislocation mobility dependence with temperature and the increase of the oxygen sub-lattice disorder in the dislocation cores is established.

Keywords: Molecular dynamics, uranium dioxide, dislocation, stacking fault

PACS: 61.72.Mm, 61.80.Lj, 61.82.Rx

*Corresponding author. Tel.: +33-1 69 08 79 15; Fax: +33-1 69 08 92 21
Email address: laurent.vanbrutzel@cea.fr (Laurent Van Brutzel)