Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Electronic Origin of Fast Sulfur Diffusion in 3d Transition Metals DMITRI NOVIKOV, UTRC, United Technologies Corporation, 411 Silver Lane, 129-21 East Hartford, CT 06108, ALAN CETEL, MICHAEL MALONEY, KEVIN SCHLICHTING, BRAD COWLES, Pratt & Whitney, 400 Main Street, East Hartford, CT 06108, SERGEY OKATOV, ILIYA LOMAYEV, YURI GORNOSTYREV, CJSC Institute of Quantum Materials Science, Ekaterinburg, Russia, SEGEI BURLATSKY, United Technology Research Center — The microscopic origins of abnormally fast diffusion of sulfur in nickel have been investigated. Transition state theory of vacancy mediated diffusion of substitutional impurities with parameters calculated from first-principle density-functional theory (DFT) was used to determinate of the diffusion coefficients of S and Al impurities in fcc Ni. Sulfur diffusion coefficient was found to be two orders of magnitude higher than for aluminum in good agreement with experimental data. We found that sulfur has a very low barrier for jump toward vacancy and also significantly decreases migration barriers for neighboring nickel atoms. We discuss the microscopic factors contributing to the dramatic difference in S and Al diffusion coefficients and show that electronic structure and chemical bonding play crucial role in enhanced diffusion of S. We also found that S considerably increases Ni self-diffusion rate. The implications of S effect on the stability of thermally grown oxides in superalloys are discussed.

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Date submitted: 14 Dec 2010 Electronic form version 1.4