Note: This is a draft of an abstract submitted for publication. Contents of this abstract should not be quoted or referred to without permission of the author(s).

To be submitted to the 2003 132nd TMS Annual International Metals and Materials Meeting and Exhibition, San Diego, California, March 2–6, 2003 (invited talk)

Impurity-Induced Grain Boundary Phase Transformations in Metals and Oxides

M. F. Chisholm[1] and G. Duscher[1, 2]

[1]Oak Ridge National Laboratory, Condensed Matter Sciences Division, Oak Ridge, TN

[2]Dept. of Materials Science and Engineering, North Carolina State Univ., Raleigh, NC

prepared by

CONDENSED MATTER SCIENCES DIVISION
OAK RIDGE NATIONAL LABORATORY
Managed by
UT-BATTELLE, LLC.
under
Contract No. DE-AC-05-00OR22725
with the
U.S. DEPARTMENT OF ENERGY
Oak Ridge, Tennessee

March 2003

2:00 PM Invited

Impurity-Induced Grain Boundary Phase Transformations in Metals and Oxides:

M.F. Chisholm[1] and Gerd Duscher [1,2]; [1]Oak Ridge National Laboratory, Condensed Matter Sciences Division, Oak Ridge, TN 37831-6030; [2]North Carolina State University, Dept. of Materials Science and Engineering, 2156 Burlington Nuclear Laboratory, Raleigh, NC 27695-7916 USA

It has been suspected that impurities can induce grain boundary phase transformations. It is difficult, however, to reveal these transformations, since to do so we must study unexpected atomic arrangements at the core of grain boundaries. This can only be accomplished by using a combination of experimental and theoretical studies with atomic resolution. In this study, we used Z-contrast imaging, electron energy-loss (EELS) and ab-initio materials simulations to study the atomic structure of grain boundaries. Z-contrast imaging provides us with directly interpretable images of the grain boundary structure, and EELS characterizes the chemical composition locally at the core of the grain boundary. The resolution of both of these techniques is greatly enhanced with objective lens aberration correction, which allows subangstrom analysis. The first results obtained with an aberration-corrected STEM are shown in this study. These experimental results allowed us to produce a starting model for ab-initio calculations. We used ultrasoft pseudopotentials and a plane wave basis set method in local density approximation. The total energies for the models with and without impurities allowed us to find the lowest energy configuration. While the grain boundary structure changed dramatically with Ca impurities in MgO, we saw only a slight modification in sigma=5 Al grain boundaries with Cu doping. However, there is no grain boundary phase transition of Cu grain boundaries with heavy dopant atoms (Bi, Ag).