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Nanoparticles in alumina: Microscopy and Theory JUAN C. IDROBO, ANDREJ HALABICA, Vanderbilt University, SERGEY RASHKEEV, Center for Advanced Modeling and Simulation, Idaho National Laboratory, MICHAEL V. GLAZOFF, Alcoa Inc., LYNN A. BOATNER, Materials Science and Technology Division, Oak Ridge National Laboratory, RICHARD F. HAGLUND, Vanderbilt University, STEPHEN. J. PENNYCOOK, Materials Science and Technology Division, Oak Ridge National Laboratory, SOKRATES T. PANTELIDES, Vanderbilt University — Transition-metal nanoparticles formed by ion implantation in alumina can be used to modify the optical properties of naturally oxidized and anodized aluminum. Here, we report atomic-resolution Z-contrast images using a scanning transmission electron microscope (STEM) of CoFe and other metal nanoparticles in alumina. We also report electron energy loss spectra (EELS) and relate them to visual appearance and optical properties. Finally, we report first-principles density- functional calculations of nucleation mechanisms for these nanoparticles. This research was sponsored by the Office of Basic Energy Sciences, Division of Materials Sciences and Engineering, U.S. Department of Energy, under contract DE-AC05- 00OR22725 with Oak Ridge National Laboratory, managed and operated by UT-Battelle, by NSF grant No. DMR-0513048, and by Alcoa Inc.

Juan Idrobo
Vanderbilt University

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