

Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Properties of Transition Metal Doped Alumina¹ ERIK NYKWEST, Univ of Connecticut - Storrs, KRISTA LIMMER, RAY BRENNAN, VICTORIA BLAIR, Army Research Lab, RAMPI RAMPRASAD, Univ of Connecticut - Storrs — Crystallographic texture can have profound effects on the properties of a material. One method of texturing is through the application of an external magnetic field during processing. While this method works with highly magnetic systems, doping is required to couple non-magnetic systems with the external field. Experiments have shown that low concentrations of rare earth (RE) dopants in alumina powders have enabled this kind of texturing. The magnetic properties of RE elements are directly related to their f orbital, which can have as many as 7 unpaired electrons. Since d-block elements can have as many as 5 unpaired electrons the effects of substitutional doping of 3d transition metals (TM) for Al in alpha (stable) and theta (metastable) alumina on the local structure and magnetic properties, in addition to the energetic cost, have been calculated by performing first-principles calculations based on density functional theory. This study has led to the development of general guidelines for the magnetic moment distribution at and around the dopant atom, and the dependence of this distribution on the dopant atom type and its coordination environment. It is anticipated that these findings can aid in the selection of suitable dopants help to guide parallel experimental efforts.

¹This project was supported in part by an internship at the Army Research Laboratory, administered by the Oak Ridge Institute for Science and Education, along with a grant of computer time from the DoD High Performance Computing Modernization Program.

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Date submitted: 04 Nov 2015

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