

Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Point defects in yttria-stabilized zirconia C. STEPHEN HELLBERG, NOAM BERNSTEIN, STEVEN C. ERWIN, Naval Research Lab — The densification that occurs during sintering of certain ceramics has been observed to occur more rapidly and at lower temperatures when a weak external electric field is applied.¹ We compute the formation energies of point defects in yttria-stabilized zirconia using first principles density functional theory. We examine interstitials, vacancies, and vacancy complexes including Schottky defects in a $\text{Y}_2\text{Zr}_{14}\text{O}_{31}$ computational cell, which corresponds to approximately 7 mol% yttria stabilized zirconia. We relate our results to recent experimental work on electric-field-assisted sintering in yttria-stabilized zirconia, showing how the expansion of lattice constants observed in diffraction measurements results from increasing defect densities. 1. Raj, R., Cologna, M., and Francis, J. S. C. Influence of Externally Imposed and Internally Generated Electrical Fields on Grain Growth, Diffusional Creep, Sintering and Related Phenomena in Ceramics. *Journal of the American Ceramic Society* **94**, 1941 (2011).

C. Stephen Hellberg
Naval Research Lab

Date submitted: 06 Nov 2015

Electronic form version 1.4