

Abstract Submitted
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Lattice Dielectric and Thermodynamic Properties of Yttria Stabilized Zirconia (YSZ) Solids¹ KAH CHUN LAU, Department of Chemistry, George Washington University, Washington D.C. 20052, BRETT I. DUNLAP, Code 6189, Naval Research Laboratory, Washington D.C. 20375 — A study of lattice dielectric and thermodynamic properties of Yttria Stabilized Zirconia (YSZ) solids as a function of yttria concentration is reported. Within the local density approximation (LDA) and the harmonic approximation, we find excellent agreement between calculated and experimental specific heat and dielectric constants. From the variation of the specific heat of YSZ with yttria composition, we propose a simple additivity rule that estimates the dependence of the specific heat of YSZ on yttria concentration. Whereas for the dielectric constants of YSZ, the values are bounded by the dielectric constants of the cubic and amorphous zirconia.

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