matter does matter

המחלקה להנדסת חומרים
אוניברסיטת בן-גוריון בנגב
Department of Materials Engineering
Ben-Gurion University of the Negev

Seminar @ Materials Engineering Department

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Extreme Anharmonicity of Chemical Bonds and Enhanced Electrostriction in Zr-Doped Ceria

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Anharmonicity of chemical bonds is responsible for many observable phenomena: thermal expansion, Raman scattering, nonlinear optics, and electrostriction, the second-order electromechanical response (strain is proportional to the square of the field: $u_3 = M_{33} \cdot E_3^2$, where M_{33} is the longitudinal electrostriction strain coefficient). The Uchino–Cross "small anharmonicity" model successfully explains the dependence of thermal expansion on elastic properties and, more importantly, accounts for Robert Newnham's empirical scaling law, which states that electrostriction scales with the ratio of dielectric permittivity (ε) to elastic modulus (Y).

In recently reported 10mol% Zr-doped ceria ($Zr_{0.1}Ce_{0.9}O_{2-\delta}$, δ=100-300 ppm, δ=100-300 ppm), the combination of $\varepsilon_3 \approx$ 200–220, and $M_{33} \approx -10^{-16}$ m^2/V^2 makes it competitive with the best commercial electrostrictor (PMN-PT15), but with ~100 times lower ε_3 and threefold higher Y. However, this combination of properties implies that under stress, σ, the change in $\Delta\varepsilon_3$ may exceed the base value: $\Delta\varepsilon_3 >> \varepsilon_3(\sigma = 0)$. This suggests that the anharmonic contribution to bond deformation energy may become comparable to, or even greater than, the harmonic component. This finding prompted us to investigate the local structure and bonding dynamics of the dopant and host bonding environments using temperature-dependent X-ray absorption fine structure (EXAFS) measurements. We found that, in addition to local disorder, there is anomalously strong anharmonicity in the Zr–O bonds, compared to Ce–O bonds. These EXAFS data explain most observed effect and suggest that by engineering the defect chemistry of Zr-doped ceria, one can create materials suitable for efficient conversion of electrical energy to mechanical energy (actuation) and vice versa (energy harvesting).

Prof. Igor Lubomirsky, the Rowland and Sylvia Schaefer Professorial Chair in Energy Research, is a professor in the Department of Molecular Chemistry and Materials Science of the Weizmann Institute of Science. I.L.'s main research interests focus on understanding the link between the structure and composition of solids with their functional properties: mechanical, dielectric, electro-mechanical, and ionic conductivity both in the bulk, at the interfaces, and on the surfaces. As a secondary field of activity, I.L. develops methods for recycling. Two of his works, in this field, recycling of Li-Co-Ni batteries and physical, rather than chemical recycling of rare-earth magnets, have reached the industrialization stage. I.L. is an active member of the Solid State Ionics Society and an editor of the corresponding journal. I.L. has published 203 works in peer-reviewed journals. Contact: Igor.Lubomirsky@weizmann.ac.il