O.30 On the calculation of electrostriction by DFT

Daniel S. P. Tanner[1,2], Pierre-Eymeric Janolin[2] and Eric Bousquet[1]

[1] *Université de Liège, Q-MAT, CESAM, Institut de Physique*
[2] *Université Paris-Saclay, CentraleSupélec, CNRS, Laboratoire SPMS, 91190 Gif-sur-Yvette, France*

Electrostriction is an electromechanical phenomenon coupling quadratically a strain or stress to an electric or polarisation field. Described by a tensor of even rank, it is present in all dielectrics. Recent measurements of very large electrostrictive coefficients [1] have generated significant interest and opened the door to electrostriction-based electro-mechanical devices. These devices will offer advantages over current piezoelectricity based technology of: reduced temperature sensitivity, low hysteresis, and lead-free materials.

In the literature, electrostriction is predominantly calculated with DFT by performing cell-relaxations under conditions of fixed electric or displacement fieldsi [2,3]. In this work we survey the existing methodologies and propose a new means by which to calculate electrostriction, which relies on the thermodynamical equivalence of the second derivatives of strain/stress with respect to electric/polarisation fields, and the first derivative of the susceptibility/inverse susceptibility with respect to strain/stress. We demonstrate, using ABINIT and DFPT, that the method produces reliable electrostrictive coefficients and has significant advantages of efficiency, clarity, robustness, and ease of use over the conventional finite-field based methods. The established method therefore allows for both high-throughput screening of materials for giant electrostriction, as well as a detailed general understanding of electrostriction, allowing for the enumeration of criteria for the design of giant electrostrictors [4].

We show applications of the method to the determination of electrostriction: in simple insulators; at a ferroelectric phase transition (KTaO3); and in ordered oxygen vacancy structures exhibiting giant electrostriction (δ-Bi_2O_3).

---

[1] R. Korobko, A. Patlolla, A. Kossoy, E. Wachtel, H. L. Tuller, A. I. Frenkel, and I. Lubomirsky, Advanced Materials **24**, 5857 (2012).

[2] I. Kornev, M. Willatzen, B. Lassen, and L. C. Lew Yan Voon, AIP Conference Proceedings **1199**, 71 (2010).

[3] C. Cancellieri, D. Fontaine, S. Gariglio, N. Reyren, A. Caviglia, A. Fête, S. Leake, S. Pauli, P. Willmott, M. Stengel, P. Ghosez, and J.-M. Triscone, Physical review letters **107**, 056102 (2011).

[4] D. S. P. Tanner, E. Bousquet, and P.-E. Janolin, Optimized methodology for the calculation of electrostriction from first-principles (2020), arXiv:2012.03841 [cond-mat.mtrl-sci].