Erratum: First-Principles Study of Piezoelectricity in PbTiO₃ [Phys. Rev. Lett. 80, 004321 (1998)]

Zhigang Wu, Gotthard Sági-Szabó, and Ronald E. Cohen

Carnegie Institution of Washington, 5251 Broad Branch Road, N.W., Washington, D.C. 20015-1305, USA

Henry Krakauer

Department of Physics, College of William and Mary, Williamsburg, Virginia 23187-8795, USA

(Received 20 December 2004; published 17 February 2005)

DOI: 10.1103/PhysRevLett.94.069901

PACS numbers: 77.84.Dy, 99.10.Cd

Tables II and IV were incorrect. In Table II the previously calculated internal displacement gradients in the second and the fourth rows were incorrect, and in Table IV all previously calculated piezoelectric stress tensor elements were incorrect except for the homogeneous part of e_{33} . The present results have been checked both with the finite strain and the strain linear response methods using the ABINIT package [1,2]. Most of the previous errors are arithmetic or transcription errors, while e_{15}^i was due to incomplete atomic relaxation.

TABLE II. Internal displacement gradients ($\sum_k \frac{\partial u_{k,i}}{\partial \epsilon_\nu} = 0$) as a function of strain.

i	ν	$\frac{\partial u_{\text{Pb},i}}{\partial \epsilon_\nu}$	$\frac{\partial u_{\text{Ti},i}}{\partial \epsilon_\nu}$	$\frac{\partial u_{\text{O}_1,i}}{\partial \epsilon_\nu}$	$\frac{\partial u_{\text{O}_2,i}}{\partial \epsilon_\nu}$	$\frac{\partial u_{\text{O}_3,i}}{\partial \epsilon_\nu}$
z	3	0.360	0.216	-0.133	-0.133	-0.310
$z, (z)$	1, (2)	0.274	-0.072	-0.148	0.131	-0.186
$y, (x)$	4, (5)	0.532	0.209	-0.391	-0.158	-0.192

TABLE IV. Piezoelectric stress tensor elements (C/m²) of tetragonal PbTiO₃.

	e_{15}	e_{31}	e_{33}
Homogeneous	1.08	-0.53	-0.88
Proper homogeneous	0.20	0.35	-0.88
Internal strain	5.45	1.52	4.56
Total	6.53	0.99	3.68
Proper total	5.65	1.87	3.68

[1] X. Gonze, J.-M. Beuken, R. Caracas, F. Detraux, M. Fuchs, G.-M. Rignanese, L. Sindic, M. Verstraete, G. Zerah, F. Jollet, M. Torrent, A. Roy, M. Mikami, Ph. Ghosez, J.-Y. Raty, and D. C. Allan, *Comput. Mater. Sci.* **25**, 478 (2002).

[2] Zhigang Wu and Ronald E. Cohen (unpublished).