AUTHOR CORRECTION OPEN

Author Correction: Strain engineering of electro-optic constants in ferroelectric materials

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After publishing this article, we realized that the calculation of the piezoelectric constants d_{ij} by Density Functional Perturbation Theory (DFPT), as explained in the methods described in the original version of the Supplementary Information, are incorrect in the case of a partially clamped situation. The correct methodology is to inverse the subspace matrix of elastic constants:

$$\begin{pmatrix} C_{33} & C_{34} & C_{35} \\ C_{43} & C_{44} & C_{45} \\ C_{53} & C_{54} & C_{55} \end{pmatrix}$$

This obtains the matrix of elastic compliances $(S_{ij})_{i,j=3,4,5}$ that applies to the mechanical directions that are unclamped in our geometry (i.e. the strains η_3, η_4 and η_5, corresponding to the relaxation of the out-of-plane axis). The relevant piezoelectric constants d_{ij} can then be calculated from: (1) the obtained reduced matrix of elastic compliances, and (2) the piezoelectric tensor e_{ij} obtained from DFPT, following the formula:

$$d_{ij} = \sum_{k=3,4,5} e_{ik} S_{kj} \quad \text{for} \quad j = 3,\ 4,\ 5$$

This correction to the methodology changes the d_{ij} calculated in Fig. 1d and Fig. 4a–d. The general findings of this work, that strain-engineering of $PbTiO_3$ films can improve electro-optic constants, is unaffected, though the size of the effect is changed.

The following corrections have been applied to the HTML and PDF versions of the article:

1. A new Supplementary Information file has been uploaded containing the above methodology in the "ELASTO-OPTIC CONSTANTS" section.
2. Following the change in methodology, Fig. 1d and Fig. 4a–d have been replaced with graphs showing the corrected data. The following sections of text have been revised due to the change in the data:

Abstract

"…via compressive strain to obtain extremely large piezo-electric constants." has been replaced with "…via compressive strain to obtain large piezoelectric constants."

Results section

"The piezoelectric constant d_{33} exhibits a strong increase to 618 p CN^{-1} at this specific strain, as shown in Fig. 1d." has been replaced with:

"As a result of this effect, the piezoelectric constant d_{33} exhibits a large increase up to 80 p CN^{-1} within the tetragonal phase, as also displayed in Fig. 1d."

"…and the large increase of the d_{33} piezoelectric constant at $\eta = -2.5\%$ (see Fig. 1d) induces very large unclamped EO constants $r_{33} \approx 95.8$ pm V^{-1} and $r_{13} = 127.1$ pm V^{-1} in Fig. 4b, c. In comparison, at zero strain, $r_{33} \approx 30.5$ pm V^{-1} and $r_{13} = 25.2$ pm V^{-1}, and a three and five time increase (with respect to the bulk case) is thus achieved under the compressive strain $\eta = -2.5\%$!" has been replaced with:

"the increase of the d_{33} piezoelectric constant at $\eta = -2.5\%$ (see Fig. 1d) induces a plateau in r_{33} and a local maximum in the r_{13} which peaks at 24.1 pm V^{-1}. More interestingly, owing to the phase-transition induced divergence of d_{33} in the monoclinic phase, the unclamped EO constant r_{33} reaches as high as 124 pm V^{-1}, which is roughly four times its clamped value and represent a four time increase with respect to the zero strain value of the unclamped EO constant in the tetragonal phase (for which $r_{33} \approx$ 30.5 pm V^{-1})."

Discussion section

"In PTO, that difference is small near the *P4mm–Cm* transition." has been replaced with:

"In PTO, that difference is small near the *P4mm–Cm* transition for the in-plane EO constants."

The following text has been added after "…without significantly affecting the EO constants in this strain region.":

"On the other hand, at the *Cm-Ic2m* phase boundary, large out-of-plane EO constants ($r_{33} \approx 124$ pm V^{-1}) can be engineered due to the strain-induced divergence of the piezoelectric constant d_{33}. The latter comes from the flattening of the energy landscape to allow for polarization rotation from the [001] pseudo-cubic direction to [110] pseudo-cubic direction [19,20]. We thus show that strain, through the exploration of phases with different symmetries, allows fine tuning of the EO constants within a single material."

"On the other hand, the large unclamped r_{33} and r_{13} of $PbTiO_3$ films…" has been replaced with:

On the other hand, the anomalous behaviors of unclamped r_{33} and r_{13} of $PbTiO_3$ films…"

"Rather, they come from the strong peak in the piezoelectric constant d_{33} seen in Fig. 1d and thus represent an original way to improve EO constants…" has been replaced with:

"Rather, they come from the strong peak in the piezoelectric constant d_{33} seen in Fig. 1d and thus represent an original way to change EO constants…"

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"At such strain, Fig. 4c reveals that the unclamped EO constant r_{33} is ≈57 pm V^{-1}, which is already twice as much as that of the standard EO material, $LiNbO_3$." has been replaced with:

"At such strain, Fig. 4c reveals that the unclamped EO constant r_{13} is ≈23.4 pm V^{-1}, which is already more than twice as much as that of the standard EO material, $LiNbO_3$ [8]."

We thank David Vanderbilt for insightful comments on this matter.