Erratum: Enhanced size-dependent piezoelectricity and elasticity in nanostructures due to the flexoelectric effect [Phys. Rev. B 77, 125424 (2008)]

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An error was found in the constitutive equations Eqs. (19) and (20) in our paper. Here we correct them. The central conclusions of our work (e.g., enhanced size-dependent piezoelectricity in nanostructures due to flexoelectricity) remain the same. In fact, corrected theoretical results in the case of $BaTiO_3$ in piezoelectric phase compare better with atomistics than in our original publication. We provide here the corrected equations and for completeness, the revised figures as well.

The correct constitutive equations are

$$\sigma_{11} = YS_{11} + dP_3 - fP_{3,3} \tag{1}$$

$$\mathrm{E}_3 = aP_3 + dS_{11} + f'S_{11,3} \tag{2}$$

By means of Poisson's equation and in the absence of free charges and applied voltage (open circuit condition) the electric displacement is

$$D_3 = \varepsilon_0 E_3 + P_3 = 0 \tag{3}$$

Equations (2) and (3) lead to:

$$-(\varepsilon_0^{-1} + a)P_3(x,z) = dS_{11} + f'S_{11,3} \tag{4}$$

Hence, the correct effective beam bending rigidity (Eq. (38) in our paper) becomes

$$G = YI\left[1 + \frac{d^2}{(\varepsilon_0^{-1} + a)Y} + \frac{Aff'}{(\varepsilon_0^{-1} + a)YI}\right] \tag{5}$$

The beam bending rigidity has the elastic, the piezoelectric, and the size dependent flexoelectric contributions.

The effective electromechanical coupling factor k_{eff} can be defined from energy consideration as the square root of the ratio of the convertible energy (electric energy) to the total input energy (mechanical energy) (see, e.g., Ref. 1 and 2).

$$k_{eff}^2 = \frac{W_{elec}}{W_{mech}} = \frac{\frac{1}{2}\int \varepsilon E_3^2 dv}{\frac{1}{2}\int YS_{11}^2 dv} \tag{6}$$

By means of Eqs. (2) and (4), the effective electromechanical coupling factor k_{eff} reduces to:

$$k_{eff} = \frac{\chi}{1+\chi}\sqrt{\frac{\varepsilon}{Y}\left(d^2 + 12\left(\frac{f\prime}{h}\right)^2\right)} \tag{7}$$

Hence, the normalized effective piezoelectric constant (with bulk piezoelectric constant) is

$$\frac{d_{eff}}{d_{piez}} = \frac{k_{eff}}{k_{piez}} = \sqrt{\left(1 + 12\left(\frac{f\prime}{dh}\right)^2\right)} \tag{8}$$

We used the flexoelectric constants values estimated by one of us[3] from *ab initio* calculations on $BaTiO_3$ (BT) as $f_{BT} = 5.46\frac{\mathrm{nC}}{\mathrm{m}}$. The piezoelectric constant of BT is taken from Ref. 4 $d_{BT} = -4.4\frac{\mathrm{C}}{\mathrm{m}^2}$.

We note that the flexoelectric constants values from *ab initio* calculations are three orders of magnitude lower than the experimental estimates reported by Cross *et al.*[5] In addition, the existence of such a large discrepancy between the *ab initio* calculations[3] and the experimental values[5] was also confirmed by the work of another independent group from Cambridge.[6] The possible reasons behind this discrepancy are discussed in details in Ref. 3.

The piezoelectric-flexoelectric interaction term incorrectly found in our paper vanishes in the revised solution. Hence, our nonpiezoelectric results in our paper remain valid and the size-dependent behavior due to pure flexoelectricity is seen at the nanoscale (in good agreement with atomistic simulations see Fig. 1). However, in the piezoelectric case (see Fig. 2), the size dependency is also due to the existence of flexoelectricity and is appreciable down to few nanometers instead of micrometers (as was found in our paper).

In Fig. 2, the effective piezoelectric response is between 3 to 4 times the bulk values at sizes around 2 nm. Our theoretical results show that the effective piezoelectric response is doubled at 2 nm and increase up to four times the piezoelectric constant

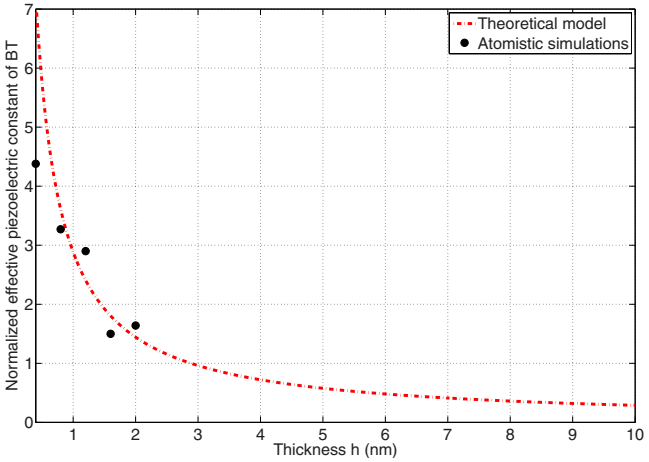

FIG. 1. (Color online) Normalized effective piezoelectric constant of cubic (non-piezoelectric) BT. The atomistic simulations are in good agreement with the theoretical model.

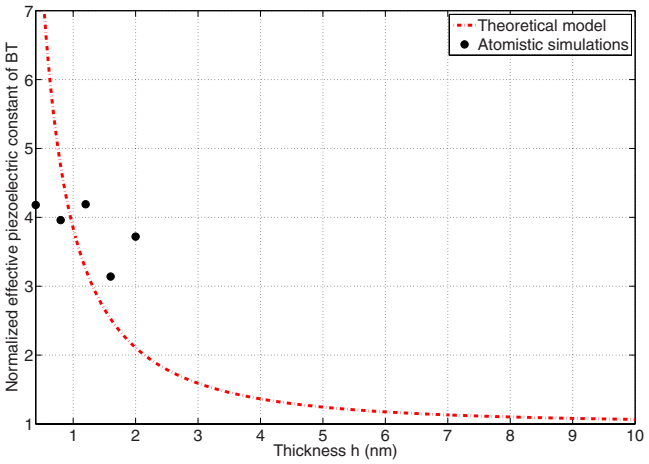

FIG. 2. (Color online) Normalized effective piezoelectric constant of tetragonal (piezoelectric) BT. The atomistic simulations are able to capture the same order of magnitude as the theoretical model. The enhancement in the piezoelectric response is seen at the nanosize.

at 1 nm. Thus, the atomistic simulations are able to capture the same order of magnitude as our theoretical results. The corrected results compare better with atomistics (see Fig. 9 in our paper). The enhancement in the piezoelectric response is significant but it is only appreciable down to few nanometers.

The results will change if flexoelectric values of Ref. 5 are used instead of first principle calculations. It is a puzzle that various atomistic models agree with each other Refs. 3 and 6 and so do experiments (Refs. 5 and 6) but atomistic models do not agree with experiments for ferroelectrics. This issue remains unresolved and meanwhile to be consistent, when comparing our theoretical results to atomistics we used the flexoelectric properties from atomistics (and likewise, comparison of various experimental results should be predicated on experimental flexoelectric values).

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