Erratum: First-principles study of pyroelectricity in GaN and ZnO [Phys. Rev. B **93**, 081205(R) (2016)]

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There was an error in Fig. 3 of this paper. The experimental temperature-dependent lattice parameters [1] $a(T)$ and $c(T)$ for ZnO were mistranscribed. This caused a significant error in the curve of Δu_{ext} . The error was not made when the derivative was plotted in Fig. 2. The results in Fig. 2 are correct, and the corrected version of Fig. 3 is given here. We also take this opportunity to add the predicted $\Delta u(T)$ for GaN, which was omitted from the original paper (the derivatives are shown in Fig. 1 of the original paper). We also wish to clarify some notations which were only implicit *via* the text but not included explicitly in the equations. The clarified version of Eq. (5) is

$$p_{\epsilon}^{\beta}(T) = \frac{e}{\Omega} \sum_{j,\kappa\alpha} Z_{\epsilon}^{\beta\alpha} \left(\frac{\partial u_{\kappa\alpha}(\vec{0}j)}{\partial T} \right)_{\epsilon},$$

FIG. 1. Corrected version of Fig. 3: Thermal shift of the ZnO internal parameter u . The measured zero temperature value is 0.382 [2,3], close to the “ideal” value of $3/8$. Experimental values are from Ref. [4]. The notation Δu_{int} refers to the computed value at constant external strain ϵ [Eq. (7)], and Δu_{ext} refers to the external strain-induced effect [last two terms in Eq. (8)].

and the wurtzite version, two lines below in the text, should read $p_{\epsilon}(T) = (2e/\Omega)Z^*c(\partial u/\partial T)_{\epsilon}$. Equation (7) is written for $\Delta u/u$, but, as the text explains, it is really $(\Delta u)_{\epsilon}/u$. The Grüneisen parameter $\gamma_{qj}^{\text{int}}(0)$ used in that equation is identified correctly in the text as the “internal” Grüneisen parameter, defined in Eq. (A14). The second term in Eq. (8) is the internal shift [it should have been written as $\Delta u_{\text{int}}(T) - \Delta u_{\text{int}}(0)$], and the last two terms are the external shift [caused by external strains $\epsilon(T)$]. Finally, recent work has clarified and extended some of this paper. A more thorough discussion on the relation between external and internal thermal expansions can be found in Ref. [5]. New measurements of $p(T)$ are now available for GaN [6]. The electron-phonon contribution, omitted in this paper, has now been computed [7] and is not negligible for ZnO or GaN.

FIG. 2. Thermal shift of the GaN internal parameter u . The derivatives du/dT were given in the original paper as Fig. 1. The notations Δu_{int} and Δu_{ext} are explained in Fig. 1.

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