

SUPPLEMENTARY DATA

Electrocaloric effect in different oriented BaZr_{0.15}Ti_{0.85}O₃ single crystals

Yun Ou¹, Chihou Lei², and Dongliang Shan^{3,*}

1. School of Materials Science and Engineering, Hunan University of Science and Technology, Xiangtan, Hunan 411201, China
2. Department of Aerospace and Mechanical Engineering, Saint Louis University, Saint Louis, Missouri 63103-1110, USA
3. Key Laboratory of Low Dimensional Materials and Application Technology of Ministry of Education, School of Materials Science and Engineering, Xiangtan University, Xiangtan, Hunan 411105, China

The thermodynamic potential energy density of the (001)-oriented bulk ferroelectric is expressed as:

$$G_{(001)}(\mathbf{E}, T) = \alpha_1(P_1^2 + P_2^2 + P_3^2) + \alpha_{11}(P_1^4 + P_2^4 + P_3^4) + \alpha_{12}(P_1^2 P_2^2 + P_2^2 P_3^2 + P_1^2 P_3^2) + \alpha_{111}(P_1^6 + P_2^6 + P_3^6) + \alpha_{112}[P_1^2(P_2^4 + P_3^4) + P_2^2(P_1^4 + P_3^4) + P_3^2(P_1^4 + P_2^4)] + \alpha_{123}P_1^2 P_2^2 P_3^2 + \alpha_{1111}(P_1^8 + P_2^8 + P_3^8) + \alpha_{1122}(P_1^4 P_2^4 + P_2^4 P_3^4 + P_1^4 P_3^4) + \alpha_{1112}[P_1^6(P_2^2 + P_3^2) + P_2^6(P_1^2 + P_3^2) + P_3^6(P_1^2 + P_2^2)] + \alpha_{1123}(P_1^4 P_2^2 P_3^2 + P_1^2 P_2^4 P_3^2 + P_1^2 P_2^2 P_3^4) - P_1 E_1 - P_2 E_2 - P_3 E_3, \quad (S1)$$

The thermodynamic potential energy density of the (110)-oriented bulk ferroelectric is expressed as:

$$G_{(110)}(\mathbf{E}, T) = \alpha_1(P_1^2 + P_2^2 + P_3^2) + \frac{1}{2}\alpha_{11}(2P_1^4 + P_2^4 + 6P_2^2 P_3^2 + P_3^4) + \frac{1}{4}\alpha_{12}(4P_1^2 P_2^2 + P_2^4 + 4P_1^2 P_3^2 - 2P_2^2 P_3^2 + P_3^4) + \frac{1}{4}\alpha_{111}(4P_1^6 + P_2^6 + 15P_2^4 P_3^2 + 15P_2^2 P_3^4 + P_3^6) + \frac{1}{4}\alpha_{112}(4P_1^4 P_2^2 + 2P_1^2 P_2^4 + P_2^6 + 4P_1^4 P_3^2 + 12P_1^2 P_2^2 P_3^2 - P_2^4 P_3^2 + 2P_1^2 P_3^4 - P_2^2 P_3^4 + P_3^6) + \frac{1}{4}\alpha_{123}(P_1^2 P_2^4 - 2P_1^2 P_2^2 P_3^2 + P_1^2 P_3^4) + \frac{1}{16}[\alpha_{1111}(16P_1^8 + 2P_2^8 + 56P_2^6 P_3^2 + 140P_2^4 P_3^4 + 56P_2^2 P_3^6 + 2P_3^8) + \alpha_{1112}(16P_1^6 P_2^2 + 4P_1^2 P_2^6 + 2P_2^8 + 16P_1^6 P_3^2 + 60P_1^2 P_2^4 P_3^2 + 8P_2^6 P_3^2 + 60P_1^2 P_2^2 P_3^4 - 20P_2^4 P_3^4 + 4P_1^2 P_3^6 + 8P_2^2 P_3^6 + 2P_3^8) + \alpha_{1122}(8P_1^4 P_2^4 +$$

* Authors to whom the correspondence should be addressed to: dlshan@xtu.edu.cn

$$P_2^8 + 48P_1^4P_2^2P_3^2 - 4P_2^6P_3^2 + 8P_1^4P_3^4 + 6P_2^4P_3^4 - 4P_2^2P_3^6 + P_3^8) + \alpha_{1123}(4P_1^4P_2^4 + 4P_1^2P_2^6 - 8P_1^4P_2^2P_3^2 - 4P_1^2P_2^4P_3^2 + 4P_1^4P_3^4 - 4P_1^2P_2^2P_3^4 + 4P_1^2P_3^6)] - P_1E_1 - P_2E_2 - P_3E_3, \quad (\text{S2})$$

The thermodynamic potential energy density of the (111)-oriented bulk ferroelectric is expressed as:

$$\begin{aligned} G_{(111)}(\mathbf{E}, T) = & \alpha_1(P_1^2 + P_2^2 + P_3^2) + \frac{1}{6}\alpha_{11}(3P_1^4 + 6P_1^2P_2^2 + 3P_2^4 + 12\sqrt{2}P_1^2P_2P_3 - 4\sqrt{2}P_2^3P_3 + \\ & 12P_1^2P_3^2 + 12P_2^2P_3^2 + 2P_3^4) + \frac{1}{12}\alpha_{12}(3P_1^4 + 6P_1^2P_2^2 + 3P_2^4 - 12\sqrt{2}P_1^2P_2P_3 + 4\sqrt{2}P_2^3P_3 + 4P_3^4) + \\ & \frac{1}{36}\alpha_{111}(9P_1^6 + 45P_1^4P_2^2 + 15P_1^2P_2^4 + 11P_2^6 + 90\sqrt{2}P_1^4P_2P_3 + 60\sqrt{2}P_1^2P_2^3P_3 - 30\sqrt{2}P_2^5P_3 + 90P_1^4P_2^2 + \\ & 180P_1^2P_2^2P_3^2 + 90P_2^4P_3^2 + 120\sqrt{2}P_1^2P_2P_3^3 - 40\sqrt{2}P_2^3P_3^3 + 60P_1^2P_3^4 + 60P_2^2P_3^4 + 4P_3^6) + \frac{1}{36}\alpha_{112}(9P_1^6 + \\ & 9P_1^4P_2^2 + 39P_1^2P_2^4 + 7P_2^6 - 18\sqrt{2}P_1^4P_2P_3 - 12\sqrt{2}P_1^2P_2^3P_3 + 6\sqrt{2}P_2^5P_3 - 48\sqrt{2}P_1^2P_2P_3^3 + 16\sqrt{2}P_2^3P_3^3 + \\ & 24P_1^2P_3^4 + 24P_2^2P_3^4 + 8P_3^6) + \frac{1}{108}\alpha_{123}(18P_1^4P_2^2 - 12P_1^2P_2^4 + 2P_2^6 - 18\sqrt{2}P_1^4P_2P_3 - 12\sqrt{2}P_1^2P_2^3P_3 + \\ & 6\sqrt{2}P_2^5P_3 + 9P_1^4P_2^2 + 18P_1^2P_2^2P_3^2 + 9P_2^4P_3^2 + 12\sqrt{2}P_1^2P_2P_3^3 - 4\sqrt{2}P_2^3P_3^3 - 12P_1^2P_3^4 - 12P_2^2P_3^4 + \\ & 4P_3^6) + \frac{1}{216}\alpha_{1111}(27P_1^8 + 252P_1^6P_2^2 + 210P_1^4P_2^4 + 28P_1^2P_2^6 + 43P_2^8 + 504\sqrt{2}P_1^6P_2P_3 + \\ & 840\sqrt{2}P_1^4P_2^3P_3 + 168\sqrt{2}P_1^2P_2^5P_3 - 168\sqrt{2}P_2^7P_3 + 504P_1^6P_3^2 + 2520P_1^4P_2^2P_3^2 + 840P_1^2P_2^4P_3^2 + \\ & 616P_2^6P_3^2 + 1680\sqrt{2}P_1^4P_2P_3^3 + 1120\sqrt{2}P_1^2P_2^3P_3^3 - 560\sqrt{2}P_2^5P_3^3 + 840P_1^4P_3^4 + 1680P_1^2P_2^2P_3^4 + \\ & 840P_2^4P_3^4 + 672\sqrt{2}P_1^2P_2P_3^5 - 224\sqrt{2}P_2^3P_3^5 + 224P_1^2P_3^6 + 224P_2^2P_3^6 + 8P_3^8) + \frac{1}{216}\alpha_{1112}(27P_1^8 + \\ & 72P_1^6P_2^2 + 150P_1^4P_2^4 + 128P_1^2P_2^6 + 23P_2^8 + 36\sqrt{2}P_1^6P_2P_3 + 60\sqrt{2}P_1^4P_2^3P_3 + 12\sqrt{2}P_1^2P_2^5P_3 - \\ & 12\sqrt{2}P_2^7P_3 + 90P_1^6P_3^2 - 630P_1^4P_2^2P_3^2 + 870P_1^2P_2^4P_3^2 - 10P_2^6P_3^2 - 420\sqrt{2}P_1^4P_2P_3^3 - 280\sqrt{2}P_1^2P_2^3P_3^3 + \\ & 140\sqrt{2}P_2^5P_3^3 + 60P_1^4P_3^4 + 120P_1^2P_2^2P_3^4 + 60P_2^4P_3^4 + 48\sqrt{2}P_1^2P_2P_3^5 - 16\sqrt{2}P_2^3P_3^5 + 160P_1^2P_3^6 + \\ & 160P_2^2P_3^6 + 16P_3^8) + \frac{1}{432}\alpha_{1122}(27P_1^8 - 36P_1^6P_2^2 + 114P_1^4P_2^4 + 188P_1^2P_2^6 + 11P_2^8 - 72\sqrt{2}P_1^6P_2P_3 - \\ & 120\sqrt{2}P_1^4P_2^3P_3 - 24\sqrt{2}P_1^2P_2^5P_3 + 24\sqrt{2}P_2^7P_3 - 72P_1^6P_3^2 + 504P_1^4P_2^2P_3^2 - 696P_1^2P_2^4P_3^2 + 8P_2^6P_3^2 + \\ & 48\sqrt{2}P_1^4P_2P_3^3 + 32\sqrt{2}P_1^2P_2^3P_3^3 - 16\sqrt{2}P_2^5P_3^3 + 96P_1^4P_3^4 + 192P_1^2P_2^2P_3^4 + 96P_2^4P_3^4 - 384\sqrt{2}P_1^2P_2P_3^5 - \\ & 128\sqrt{2}P_2^3P_3^5 + 64P_1^2P_3^6 + 64P_2^2P_3^6 + 16P_3^8) + \frac{1}{108}\alpha_{1123}(18P_1^6P_2^2 + 6P_1^4P_2^4 - 10P_1^2P_2^6 + 2P_2^8 - \\ & 18\sqrt{2}P_1^6P_2P_3 - 30\sqrt{2}P_1^4P_2^3P_3 - 6\sqrt{2}P_1^2P_2^5P_3 + 6\sqrt{2}P_2^7P_3 + 9P_1^6P_3^2 + 45P_1^4P_2^2P_3^2 + 15P_1^2P_2^4P_3^2 + \\ & 11P_2^6P_3^2 - 6\sqrt{2}P_1^4P_2P_3^3 - 4\sqrt{2}P_1^2P_2^3P_3^3 + 2\sqrt{2}P_2^5P_3^3 - 3P_1^4P_3^4 - 6P_1^2P_2^2P_3^4 - 3P_2^4P_3^4 + 12\sqrt{2}P_1^2P_2P_3^5 - \\ & 4\sqrt{2}P_2^3P_3^5 - 8P_1^2P_3^6 - 8P_2^2P_3^6 + 4P_3^8) - P_1E_1 - P_2E_2 - P_3E_3 \quad (\text{S3}) \end{aligned}$$