Piezoelectric constants of $KNbO_3$ by molecular dynamics simulations using a shell model

T. Hashimoto[1], H. Moriwake[2]

[1]Nanosystem Research Institute (NRI), National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba Central 2, 1-1-1 Umezono, Tsukuba, Ibaraki 305-8568, Japan
[2]Nanostructures Research Laboratory, Japan Fine Ceramics Center, 2-4-1 Mutsuno, Atsuta-ku, Nagoya, 456-8587, Japan

$KNbO_3$ is an ABO_3 type perovskite whose solid solution with other A site atoms could be a potential candidate for Pb free piezoelectric materials. $KNbO_3$ undergoes phase transitions among, listing from high temperature to low temperature, cubic (C), tetragonal (T), orthorhombic (O), and rhombohedral (R) phases. Despite its importance, the number of the experimental reports on the piezoelectric constants of $KNbO_3$ is small due to the difficulty in the growth of high quality crystals and in the poling treatments, and these reports are limited to room temperatures. In this paper, we predicted the temperature dependence of the piezoelectric coefficients of $KNbO_3$ by molecular dynamics simulations using a shell model[1].

The piezoelectric constants were calculated by[2-4]

$$d_{kij} = \left(\frac{\partial \eta_{ij}}{\partial E_k}\right)_{\sigma,T} = \frac{1}{k_B T} \langle \Delta M_k \Delta \eta_{ij} \rangle .$$

Here, η, $\mathbf{E}$, σ, T, k_B, and $\mathbf{M}$ are the strain tensor, the electric field, the stress, the temperature, the Boltzmann's constant, and the total dipole moment of the MD cell, respectively. ΔX represents X - $\langle X \rangle$, where X is M_k or η_{ij}.

Figure 1 shows the temperature dependence of piezoelectric coefficients d_{ij} for $KNbO_3$ in all three ferroelectric phases. The results were similar to those by the Landau-Ginzburg-Devonshire (LGD) theory[5] and the first-principles calculations for the R phase[6] of $KNbO_3$. The shear and some of the longitudinal piezoelectric constants changed by 200 ― 300 % depending on the temperature. This is because the dipole moment deviation from its average value and the strain deviation from its average value are greatly dependent on temperatures. So, it should be difficult to predict the piezoelectric constants by first-principles calculations except for the R phase.

We also predicted the temperature dependence of the longitudinal piezoelectric surface d^*_{33} of $KNbO_3$. The results were also similar to the previous calculations, since the temperature dependence of the piezoelectric constants were similar to them. Near the T-C phase transition temperatures, due to the enhanced d_{33}, d^*_{33} is large along the polar direction. For other temperatures, especially near the phase boundaries, the large shear piezoelectric constants result in the maximum of d^*_{33} along the non-polar directions.

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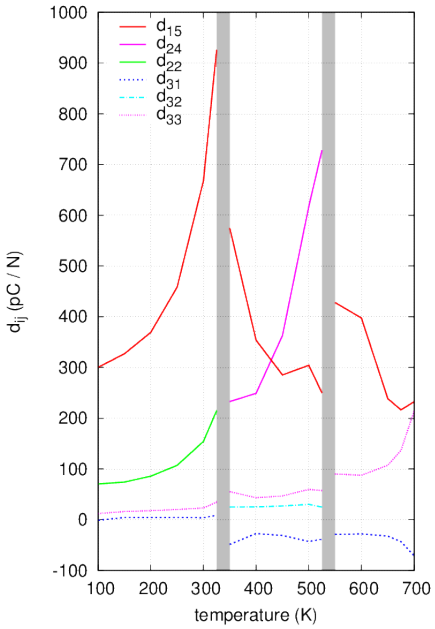

Figure 1. Piezoelectric coefficients for $KNbO_3$.

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