Defect-polarization control for enhancing piezoelectric properties of $BaTiO_3$-based single crystals and ceramics

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The properties of ferroelectric materials are governed by domain (polarization) structures and their dynamics with respect to external stimuli. It has been reported that engineered domain configurations with a fine domain structure enhance piezoelectric and dielectric properties.[1-3] These enhanced properties are suggested to originate from a large response with electric field (E) around domain-wall (DW) regions.[2] It has been reported that charged DWs show a giant dielectric and piezoelectric response with E.[4]

One of the other intriguing characteristics of ferroelectrics is a photovoltaic effect. The photovoltaic charge separation has been reported to operate near the ferroelectric DWs with a distance of 1–2 nm. [5]

The defect-polarization control is defined as the domain engineering based on defect chemistry. This concept originates from the strong attractive interaction between ferroelastic DWs and oxygen vacancies ($V_O^{\bullet\bullet}$). [6-8] Our DFT calculations show that the energy of 90° DWs in $PbTiO_3$ is largely reduced by introducing $V_O^{\bullet\bullet}$ from 37 mJ/m^2 (perfect crystal) to 11 mJ/m^2 ($PbTiO_{2.833}$). In this study, $BaTiO_3$ (BT) single crystals are chosen as model materials and the doping of an acceptor of Mn is selected as a means for introducing $V_O^{\bullet\bullet}$ into BT.

Figure 1 (a) shows the piezoelectric strain coefficients (d) (the slope of S at low E's along <110>) as a function of Mn content (x). Mn (0.1 %)-BT showed a d of 630 pm/V, which was much larger than that of undoped BT (69 pm/V) and single domain BT crystals (86 pm/V[7]). Figure 1 (b) shows the piezoresponse-force microscope (PFM) image (in-plane, phase) of Mn (0.1 %)-BT crystals poled along <110>. Mn-BT had a peculiar domain structure with a size of 20 ~ 40 nm. This domain size was much smaller than that of undoped BT poled along <110> (0.02 ~ 0.03 mm). These results show that the domain size of BT-based crystals became much smaller by the Mn doping.

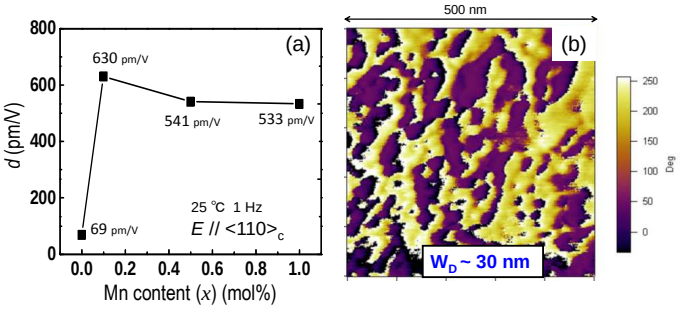

Fig.1. (a) Piezoelectric strain coefficient (d) as a function of Mn content (x) and (b) PFM phase image (in-plane) of Mn(0.1 %)-BT crystals poled along the <110> direction.

References

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