

K. Golasinski, E. Piecyska, M. Maj, M. Staszczak, N. Takesue, *Plastmet 2016, Jubileuszowe X Seminarium Naukowe ZINTEGROWANE STUDIA PODSTAW DEFORMACJI PLASTYCZNEJ METALI*, Lancut, Poland(2016-11-22/11-25).

Evaluation of Ionicity/Covalency of Atoms in Barium titanate with Barium Replaced by Bismuth and Lanthanum / N. Takesue, K. Ishibashi and K. Asakura (Fukuoka Univ.) / Research and development of lead-free perovskite ferroelectrics, traditionally designated as ABO_3 , have been a subject of the harmless application since many years ago. This trend seems to stay around the stage of the bismuth- or lanthanum-replaced systems for the last several years, which was motivated us to investigate ionicity/covalency for the type of system with first-principle cluster calculation. The results show appreciable covalent bonding between bismuth and oxygen, and also lanthanum and oxygen. This feature is quite similar to the covalency between lead and oxygen in lead titanate, which was considered only one exclusively good component for the high performance, and suggests that the replacement is effective. The Ceramic Society of Japan, Annual Meeting, March 17th-19th.

Experimental study of solid solutions of bismuth-sodium titanate BNT based on their simulated ionicity/covalency. / K. Asakura, Y. Asano, N. Takesue (Fukuoka Univ.), Z. Xu, K. Matsugi (Hiroshima Univ.) / We fabricated perovskite ABO_3 ferroelectric solid-solution systems, which is based on our previous first-principles cluster calculation; the fabrications were done by flux powder sintering. Crystal structures of the samples were investigated by X-ray diffraction; (200) Bragg reflections of the typical primitive cell were monitored carefully. The results of, e.g. $(Bi_{1/2}Na_{1/2})TiO_3$ - $BaTiO_3$, show a possible morphotropic feature over phase states of the tetragonal and rhombohedral structures. We expect that the effect will provide the excellent piezoelectric properties. We will present systematic results of these measurements. The Ceramic Society of Japan, The 30th Fall Meeting, Sept. 19th-21st.