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Surface properties of ultrathin ferroelectric films in external electric field RENAT SABIRIANOV, University of Nebraska at Omaha, MINORU OTANI, National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Japan, OSAMU SUGINO, University of Tokyo — The electric polarization of free standing ultrathin films of $BaTiO_3$ is analyzed using pseudopotential plane wave calculations within effective screening medium method. The polarization loop in asymmetrically terminated (Pb,Ba)TiO_3 film is biased, providing the existence of polarization without applied electric voltage across the film. We attribute the origin of bias to a creation of a bias field due to difference in surface work functions of TiO_2 and BaO terminations. This results in the formation of surface polarizations at each termination and inhomogeneous polarization profile across the thickness of the film. We show that the surface develops in-plane component of polarization in paraelectric state, and also in case of the ferroelectric films when the electric field applied perpendicularly to the plane of the film.

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