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Strain-mediated $SrTiO_3/PbTiO_3$ superlattice: The role of oxygen vacancy MENGLEI LI, WENHUI DUAN, Tsinghua University — Using first-principle calculations, we comprehensively study the oxygen vacancy effects on the ferroelectric(FE) and antiferrodistortive(AFD) properties of the [001]-oriented $SrTiO_3/PbTiO_3$ 1/1 superlattice at different epitaxial strains. Oxygen vacancies form most easily under intermediate strains while the oxygen on the PbO-plane is more difficult to lose than in other positions. Without vacancies, the superlattice is in the r-phase where the polarization has both in-plane and out-of-plane components at intermediate strain. The oxygen vacancy can pin the polarization to the out-of-plane direction and remarkably reduce the polarization in the direction of Ti-V_O-Ti chain by inducing local tail-to-tail polarization patterns. Furthermore, the oxygen vacancies suppress the octahedra rotations around the direction of Ti-V_O-Ti chain while promote the rotations along the other two orthogonal directions. Therefore, the mediation of the FE and AFD properties in different directions in the superlattice can be achieved by the use of the anisotropic effect of oxygen vacancies. Our results provide a theoretical ground to the various coupling effects in ferroelectric-paraelectric superlattices.

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