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Manifestation of bilinear flexo-antiferrodistortive coupling at twins and antiphase boundaries in ferroelastics

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The flexoelectric-type coupling between the gradients of electric polarization, described by a true polar vector $\vec{P}$, and the antiphase rotation of structural groups, described by an axial pseudovector $\vec{\Phi}$, can lead to the appearance of interfacial polarization at the twin walls, antiphase boundaries and surfaces of antiferrodistortive (AFD) ferroelastics [1]. The linear-quadratic flexo-AFD coupling may contribute significantly to observable interfacial polarization induced by oxygen octahedral rotations at the antiphase boundaries and/or twin walls in YMnO3, Ca3Mn2O7, CaTiO3 and SrTiO3, as well as lead to the appearance of versatile spatially modulated structures in multiferroics [1].

The quadratic dependence of the linear-quadratic flexo-AFD coupling energy on $\vec{\Phi}$ appeared principally important for the emergence of interfacial polarization, because the odd powers of anti-phase (i.e., sign-alternating in neighboring sublattices) pseudovector $\vec{\Phi}$ cannot induce the continuous polarization of structural domain walls, surfaces or interfaces in AFD ferroelastics. Therefore, it seemed that it made little sense to consider odd powers of $\vec{\Phi}$ when constructing the sublattice-insensitive flexo-AFD coupling energy. However, recently Visser et al. [2] and Fang et al. [3] proposed the concept of alterelectricity, an electrical analogue of altermagnetism, in which two switchable states possess alternating band structures.

Using the Landau-Ginsburg-Devonshire approach we show that the linear gradient-type coupling between the electric polarization vector $\vec{P}$ and antiferrodistortive long-range order parameter pseudovector $\vec{\Phi}$, that has the form of Lifshitz invariant $\left(\vec{P} \bullet \nabla \times \vec{\Phi} \; - \vec{\Phi} \bullet \nabla \times \vec{P}\right)/2$ and named "bilinear flexo-antiferrodistortive coupling", can emerge in all antiferrodistortive ferroelastics, since it is symmetry-allowed [4]. Using the four sublattices model we reveal that the bilinear flexo-antiferrodistortive coupling can induce the sublattice-sensitive polarization at the twin walls and antiphase boundaries in antiferrodistortive ferroelastics without any ferroelectric or antiferroelectric ordering. Since the induced polarization $\delta\vec{P}$ is perpendicular to $\vec{\Phi}$ and counter-directed in neighboring sublattices with checkerboard-type direction of $\vec{\Phi}$, such structure of $\delta\vec{P}$ may correspond to the alterelectric-type quadrupolar electric order. However, physical manifestations of the bilinear flexo-antiferrodistortive coupling are invisible in most nanostructured antiferrodistortive ferroelectrics and antiferroelectrics due to the domination of piezoelectric and/or omnipresent linear flexoelectric couplings. We have shown that the bilinear flexo-antiferrodistortive coupling can induce alterelectric-type polarization near antiferrodistortive domain boundaries in ferroelastics without any ferroelectric or antiferroelectric long-range ordering [1].

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