Piezomagnetic effect in Mn-based antiperovskites

RENAT SABIRIANOV, PAVEL LUKASHEV, University of Nebraska, Omaha, KIRILL BELASHCHENKO, University of Nebraska, Lincoln — We predict large piezomagnetic effect in Mn-based antiperovskites. The magnetic ground state is determined to be the non-collinear $5g$ structure, which can be viewed as a sequence of alternating layers of clockwise and counterclockwise triangular spin currents in (111) plane, resulting in the zero total magnetization of the system. We use PAW method (VASP) within PBE generalized gradient approximation. We find that the system develops non-zero magnetization under biaxial strain due to the lowering of the crystal symmetry from cubic to tetragonal. The system exhibits linear magnetization dependence on the applied strain over the moderate range (up to 1%) of the latter. The magnetization under strain appears as a result of the rotation of local magnetic moments (LMM) on Mn atoms in Mn$_2$N plane. Besides, the system exhibits biaxial anisotropy under strain. We propose using the observed piezomagnetic effect to build the magnetoelectric perovskite ferroelectric – antiperovskite piezomagnetic heterostructures. The estimated magnetoelectric coefficient is $\sim 2\times10^{-9}$s/m. Because of the piezomagnetic effect, Mn-based antiperovskites can be used in memory cells with electric control of magnetization. It can be also applicable in spintronics, as the system develops a net polarization of up to 30% under external strain.

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