Symmetry and Structure of $SrTiO_3$ Nanotubes

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The line symmetry group $L=ZP$ (a product of one axial point group P and one infinite cyclic group Z of generalized translations) of single-walled (SW) and double-walled (DW) $SrTiO_3$ nanotubes (NT) is considered. The nanotube is defined by the square lattice translation vector $\mathbf{L} = l_1\mathbf{a} + l_2\mathbf{b}$ and chiral vector $\mathbf{R} = n_1\mathbf{a} + n_2\mathbf{b}$, ($l_1$, l_2, n_1 and n_2 are integers). The nanotube of the chirality (n_1, n_2) is obtained by folding the (001) layer (with the layer group P4*mm*) in a way that the chiral vector **R** becomes circumference of the nanotube.

For SW (n,0) NTs the line symmetry groups belong to family 11 (T^D_{nh}) and are n/mmm or $\overline{2n}\,2m$ for even and odd n, respectively. For SW (n,n) NTs the line symmetry groups $(2n)_n/mcm$ belong to family 13 ($T_{2n}{}^1D_{nh}$).

The line symmetry group of a double-wall nanotube can be found as intersection $L_2 = Z_2P_2 = (L \cap L')$ of the symmetry groups L and L' of its single-wall constituents as earlier considered for DW CNTs [1,2].

In particular case of the commensurate (n,n)@M(n,n) and (n,0)@M(n,0) DW perovskite nanotubes with square morphology the DW NT symmetry group depends on the parity of M. For DW NTs with odd M, the line symmetry groups are the same as for their SW constituents and belong to families 13 and 11 respectively. For even M, the rotations about screw axis of order $2M$ are changed by rotations around pure rotation axis of order M so that DW NT line symmetry groups belong to family 11 for both chiralities.

The results of the first principles LCAO-PBE0 calculations of SW and DW $SrTiO_3$ NTs are presented. CRYSTAL-09 computer code [3] is used, the rod subgroups of line groups are applied allowing the large scale computations for NTs. The DW nanotubes strain energy is estimated relatively to the sum of their constituents energies.

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References

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