Ferrodistortive lattice modes and polytypism in LaO$_{1-x}$F$_x$BiS$_2$ superconductor

ANUSHIKA ATHAUDA, DESPINA LOUCA, Univ of Virginia, CHRISTINA HOFFMAN, Oak Ridge National Laboratory, YANG REN, Argonne National Laboratory, XIANGDE ZHU, SAICHARAN ASWARTHAM, JASMINKA TERZIC, GANG CAO, Univ of Kentucky — LaO$_{1-x}$F$_x$BiS$_2$ is a disordered, non-magnetic superconductor with a transition temperature of 10.8 K at $x = 0.5$. The crystal structure of LaO$_{1-x}$F$_x$BiS$_2$ is investigated using synchrotron X-ray and neutron diffraction experiments. The Bragg pattern obtained in hk0 plane could not be reproduced by either the long-presumed nominal symmetry P4/nmm or other theoretically suggested symmetries and indicated the possibility that the symmetry is lower than expected. The Bragg structure can be reproduced by a model involving coordinated ferrodistortive in-plane displacements of sulfur. Several possibilities of sulfur displacement arrangements can reproduce the data equally well leading to the possibility of domains. When several domains are averaged together the fitting results improve. Therefore, the structure most likely consists of polytypes stacked along the c-axis. In the superconducting planes, the structure needs to be uniform, otherwise domain walls are created due to antiferrodistortive arrangements, giving rise to additional peaks not present in the data.

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