Fluorine doping of barium bismuthate for topological qubits

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Quantum computing promises to greatly decrease the time required to solve problems that benefit from parallel computation, with applications in many different fields such as cryptography, machine learning, logistics or drug development. At the core of a quantum computer there are the qubits, systems in which a superposition of two states can be precisely prepared and manipulated. In the literature many different proposals for physically realizing a qubit can be found, each one with its own advantages and disadvantages. Among them, we can find topological qubits. Instead of being based on a two-level system like most of the other qubits, topological qubits would use the physical braiding of non-abelian anyons, particles that pick up a phase shift different than π or 2π when exchanged, to execute quantum computations. In this way, the impact of the major obstacle to quantum devices, the decoherence of the qubits due to their interaction with the environment, could be drastically decreased [1]. Theoretically, one approach to realize topological qubits is through the deposition of superconductive (SC) islands on a topologically insulating (TI) continuous film. [2]

A very promising material for this approach is barium bismuthate ($BaBiO_3$, BBO), a perovskite expected to behave both as a SC and a TI, depending on the doping, allowing the realization of high-quality SC-TI heterostructures. In particular, p-doped BBO is a well-known SC with a critical temperature up to 30K [3], while n-doped BBO (*e.g.* by substituting the oxygen with fluorine atoms), is expected by ab-initio DFT to be a TI [4]. Furthermore, the topological bandgap of BBO is expected to be around 0.7 eV [4], higher than the other TIs extensively studied in the literature like Bi_2Se_3, Bi_2Te_3 or Bi_xSb_{1-x} [5], further improving the quality of a BBO based-topological qubit.

Despite its potential, the realization of a TI BBO is still an open question in the literature. Here we report our attempts at introducing fluorine into the structure of 20nm-thick MBE-grown epitaxial BBO thin films on grown on Si (001) through an STO buffer layer. From the literature, we expected oxygen deficient perovskites to be more efficiently fluorinated [6], thus, we also investigated the effect of the process on oxygen deficient films. As fluorinating agent, we chose plasma of a gas commonly found in semiconductor facilities: SF_6.

After finding processing conditions for which the film' integrity is conserved, we studied the effect on crystallinity by XRD and composition by XPS and SIMS. By XRD we were able to assess an increase in the out-of-plane lattice parameter in the BBO samples. By XPS, a clearly visible F 1s core level peak, with a component compatible with the formation of a metal fluoride was detected. Finally, SIMS investigation allowed us to further confirm an increase of fluorine into the processed samples coupled to a decrease in oxygen concentration. In SIMS data we also saw a higher concentration of fluorine in the oxygen deficient samples, confirming our initial hypothesis. All these results seem to indicate at least a partial substitution of oxygen with fluorine in the BBO samples. We also performed a second anneal in oxygen on some of the fluorine samples and observed an increase in crystallinity and a decrease in the lattice parameter by XRD, suggesting a partial reversibility in the process.

In the future a more detailed investigation on the structure by TEM and an investigation of the impact on the transport properties will be carried out.

References

1. S. Das Sarma, M. Freedman, and C. Nayak, Phys. Rev. Lett. 94, 166802 (2005)
2. L. Fu and C. L. Kane, Phys. Rev. Lett. 100, 096407 (2008)
3. H. Yamamoto, K. Aoki, A. Tsukada, and M. Naito, Physica C 412-414, 192 (2004)
4. B. Yan, M. Jansen, and C. Felser, Nat. Phys. 9, 709 (2013)
5. J. Yun and L Xi, Adv. Quantum Technol. 7, 2400041 (2024)
6. O. Clemens and P. R. Slater, Rev Inorg Chem, 33, 105 (2013)

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