Monte Carlo analysis of the oxygen knock-on effects induced by synchrotron x-ray radiation in the $Bi_2Sr_2CaCu_2O_{8+\delta}$ superconductor

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We investigate the microscopic mechanism responsible for the change of macroscopic electrical properties of the $Bi_2Sr_2CaCu_2O_{8+\delta}$ high-temperature superconductor induced by intense synchrotron hard x-ray beams. The possible effects of secondary electrons on the oxygen content via the knock-on interaction are studied by Monte Carlo simulations. The change in the oxygen content expected from the knock-on model is computed convoluting the fluence of photogenerated electrons in the material with the Seitz-Koehler cross section. This approach has been adopted to analyze several experimental irradiation sessions with increasing x-ray fluences. A close comparison between the expected variations in oxygen content and the experimental results allows determining the irradiation regime in which the knock-on mechanism can satisfactorily explain the observed changes. Finally, we estimate the threshold displacement energy of loosely bound oxygen atoms in this material $T_d = 0.15^{+0.025}_{-0.01}$ eV.

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I. INTRODUCTION

The study of the interaction between radiation and materials has been the subject of intense efforts in the past, clarifying many aspects of the fundamental mechanisms involved [1] and considering several classes of materials ranging from diamond [2] to high-temperature superconductors (HTSCs) [3]. Focusing on HTSCs, it is well known that swift heavy ions induce well-defined columnar tracks, consisting of amorphized material [4,5], which are very effective in preventing the vortex movement and therefore in increasing the critical current [6–9]. This is due to the good matching between both shape and size of the amorphous tracks and the vortexes, which does not occur in the case of proton irradiation, because it only generates localized cascades of defects, inducing a much less effective vortex pinning [10,11].

The effect of electron irradiation has also been investigated in these materials, highlighting the formation of pointlike defects [12] that cause a decrease of the critical temperature T_c and an increase of the normal state resistivity both in $YBa_2Cu_3O_{7-x}$ [13] and in $Bi_2Sr_2CaCu_2O_{8+\delta}$ (Bi-2212) [14], where energy dependent structural modifications were also observed [15].

Photons are also known to change the properties of HTSCs. For instance, γ-ray irradiation was shown to reduce T_c in Bi-based superconductors [16] and to suppress the supermodulation of Bi-2212 [17]. Concerning x rays, it is well known that intense synchrotron beams can alter the state of the materials, but this effect is generally considered undesired radiation damage. However, interesting effects that in principle could be useful to modify materials in a controlled way, have been reported in the past [18], including for instance redox reactions [19], metal-insulator [20], and structural phase transitions [21]. Also in the case of HTSCs the irradiation with synchrotron hard x rays has been reported to modify the normal and the superconducting properties of the target material [22,23], and this fact has recently been exploited to produce functioning electronic devices out of Bi-2212 single crystals by means of a novel nanopatterning technique [24,25]. However, the precise microscopic mechanism linking intense x-ray irradiation to the macroscopically observed properties modifications has not been clarified yet. A deeper understanding would improve the general knowledge in the field of photon-induced damage and could facilitate the optimization of this nanopatterning technique and its extension to other materials.

Since the electronic properties of superconducting oxides critically depend on the concentration of loosely bound excess oxygen atoms, a possible origin of this effect could rely on the secondary electrons produced by the x-ray beam, which could induce atom displacement via knock-on interaction.

In recent years, an approach based on Monte Carlo simulations was proposed by Piñera *et al.* [26] to evaluate the importance of the knock-on mechanism in the damage of $YBa_2Cu_3O_{7-x}$ by γ radiation, showing that non-negligible fractions of oxygen atoms can be displaced if the threshold energy for this phenomenon is low enough.

The present paper is intended to further develop this approach and interpret some recent experimental results [22,24] concerning the irradiation of Bi-2212 microcrystals with a hard x-ray synchrotron nanobeam. The comparison between modeling and experimental results is expected to clarify whether

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