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Monte Carlo simulation of vacancies produced in lead-free piezo-ceramics by X-ray radiation damage

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Abstract

Fourth-generation synchrotrons, such as ESRF – EBS (Extremely Brilliant Source) have a very high brilliance of 5x1022 photons / s / mm2 / mrad2 / 0.1% BW. This light is produced in pulses of very short duration, which allows experiments with high spatial, energetic and temporal resolutions. However, high brilliance produces huge beam intensities. This leads us to investigate whether the samples with a medium atomic number can be damaged during the experiments in the fourth-generation synchrotrons 1. These could be the case of experiments on ferroelectric materials. Radiation damage in ferroelectrics is reported in the literature. Among the consequences of ionizing radiation damage is the production of vacancies. Most of the studies have been carried out in PZT and using intense beams of X-rays, whose energy is much higher and the probability of interaction much lower than X-rays 2. This work presents the preliminary results of a simulation by the Monte Carlo method, performed through the GEANT4 code, of the irradiation of a BNBT6 ceramic with X-rays energies around the Ti-K absorption edge emulating a transmission experiment, and irradiation with 5300 eV X-rays for fluorescence measurement. The method consists of introducing the data that describe a characteristic R3c structure of the polarized ceramic, reported at Canche et al. 3. The absorption coefficients for the energies of interest, as well as the energy deposited in the form of radiation doses, are calculated. Intensity changes for specific energy lines in the micro-fluorescence spectra, which suggest the presence of vacancies in the crystal structure, are verified via simulation. The vacancy density produced by a typical photon flux of a fourth-generation synchrotron beam is calculated through the vacancy formation energy. Consequently, the simulation is carried out for a structure with appropriate Bi and O vacancies, and the ability to detect the radiation damage is verified by comparison with XRF and XAFS experimental results 3. The support provided by Project CONACYT Projects No. 183706 and 257912, as well as MINECO MAT2017-86168-R, Spain, is acknowledged. A part of the experiments was performed (as part of Proposal No. 3511) at the Stanford Synchrotron Radiation Lightsource (SSRL). XAFS experiments were accomplished at the European Synchrotron Radiation Facility (ESRF) at Grenoble, as part of the proposal HG/77.

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