Structural Symmetry in Pulsed Laser Deposited Niobium-Lead Germanate Thin Films by DFT and XAFS

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Nb_2O_5-PbO-GeO_2 (NPG) glasses are promising candidates for applications in nonlinear optical devices because they exhibit high nonlinear third order optical susceptibility. Previously, it was shown that oxygen stoichiometry has a very important effect to produce unusual high optical susceptibility. The crystal structure of NPG) glass thin films on silicon substrates were investigated by using XAFS and Density functional theory (DFT) based simulated standards. In this work NPG glasses were prepared with pulsed laser deposition (PLD) method with varying oxygen partial pressure to induce thin films with different oxygen stoichiometry. In our study of these materials, we have discovered interesting crystal structure responses to partial oxygen deposition pressure[1]. In this study, we have prepared a series of Nb_2O_5-PbO-GeO_2 glasses on Si substrates under various oxygen partial pressures from vacuum to 5Pa. Glancing incidence EXAFS and measurements were performed at Brookhaven National Laboratory. Then we have used DFT based calculated references and experimental references to identify the crystal phases present in the thin films prepared with various partial oxygen pressures. The results of the EXAFS non-linear square fits will be presented to correlate the PLD deposition parameters to the final phases obtained in these thin films.

1. Sahiner et al., Journal of Physics 712, 012103 (2016).

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