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Pulsed laser ablation I : Maria Dinescu

[Determination of Structural Symmetry in Niobium Germanate Thin Films by DFT Assisted EXAFS Analyses](#)

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09:00 Resume : The crystal structure of Niobium-lead-germanate, Nb₂O₅-PbO-GeO₂ (NPG), glass thin films on silicon substrates were investigated by using EXAFS and Density functional theory (DFT) based simulated standards. NPG glasses are promising candidates for applications in nonlinear optical devices because they exhibit high nonlinear third order optical susceptibility. 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 pressure¹. In this study, we have prepared a series of Nb₂O₅-PbO-GeO₂ 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 discussed 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).