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Topic: Structural, Optical and Mechanical Analyses of Technologically Important Nonlinear Optical Single Crystals

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This research provides a comprehensive view of the nonlinear optical (NLO) material. lithium niobate (LiNbO3) single crystal. Through meticulous analysis of crystal growth techniques, particularly the Czochralski method from melt, this study aims to fabricate high-quality bulk single crystals of $LiNbO_3$.

1. This thesis work is mainly focused on the analysis of certain single crystals of doped and undoped $LiNbO_3$; the properties and crystalline perfection as a function of dopant concentration is studied
2. The investigation delves into the transformative effects of doping with elements such as Ruthenium (Ru), Magnesium (Mg), Zinc (Zn), and Iron (Fe) on the optical, mechanical, and structural properties of $LiNbO_3$
3. Ruthenium (Ru) and magnesium (Mg) co-doping in $LiNbO_3$ single crystals grown via the Czochralski method demonstrated good crystalline quality, statistically distributed dopants, and enhanced polarisability, leading to high optical transparency and a shift in absorption edge towards shorter wavelengths.
4. Ru-Mg Co-doping influenced electronic band-gap energies, resulting in reduced refractive indices and increased band gap energy, while second harmonic generation (SHG) efficiency decreased with higher Ru: Mg concentrations.
5. The study investigated the structural properties of magnesium (Mg)-doped lithium niobate (LN) single crystals using X-ray diffraction (XRD) and Raman spectroscopy. Increasing Mg content led to a slight increase in lattice parameters and lattice strain.
6. Mechanical properties were assessed through nanoindentation, revealing that optimal Mg doping levels enhanced mechanical strength, as indicated by higher Young's modulus and hardness values, highlighting increased rigidity and strength of the crystals.
7. Co-doping lithium niobate (LN) crystals with Zn and Fe influenced their optical properties, as UV-Vis-NIR spectral analysis showed transparency from 375 to 1200 nm, with a lowered band gap due to co-doping.
8. Raman spectra indicated minimal changes in lattice vibrational modes with Zn and Fe addition, suggesting no fundamental structural alterations. The two-beam coupling experiment demonstrated a diffraction efficiency of 62.29%, highlighting the material's suitability for photorefractive applications due to its sensitivity and efficient diffraction properties.