

Effect of Oxygen Flow Rate on the Lattice Spacing and Oxygen Composition of ZnTeO Epitaxial Layers Grown on GaAs (001) by MBE

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ZnTeO is a highly promising photovoltaic material due to its tunable bandgap and superior optical properties, enabling the achievement of high photoelectric conversion efficiency. [1] To investigate the influence of oxygen substitution on the lattice spacing and chemical composition of ZnTe layer, this study employed molecular beam epitaxy (MBE) to grow ZnTeO layers approximately 300 nm thick on GaAs (001) substrates under varying oxygen flow rates.

The crystal in the growth layer will be strained, and the lattice spacing will not be the same in the growth direction and the in-plane direction. To analyze strained crystals, the undistorted lattice spacing a_0 is calculated by using in-plane lattice spacing a_{\parallel} and vertical lattice spacing a_{\perp} . The lattice spacing of the layers were measured by reciprocal lattice mapping of ZnTeO (224) using XRD. Results in Fig. 1 showed a slight fluctuation in lattice spacing, with oxygen flow rate increasing. This trend suggests that oxygen substitution has a minimal direct impact on the crystal lattice structure, likely inducing local lattice expansion or defect formation.

The relationship between lattice spacing and oxygen flow rate during growth, as shown in Fig. 2, reveals how oxygen incorporation affects crystal structure and strain, providing insights for material optimization. The oxygen composition was calculated based on the lattice spacing and Vegard's law under the assumption of no distortion calculated earlier. It was found that it contains up to 1.2% oxygen. In some samples, the results are not very satisfactory. This is believed to be due to the deterioration of crystallinity with each increase in oxygen flow rate and the thinning of the film thickness, making it difficult to read the peak position.

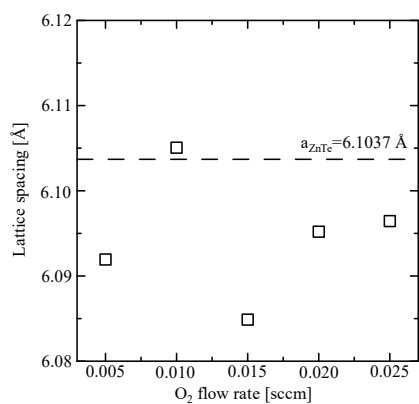


Fig. 1 Relationship between lattice spacing and O₂ flow rate.

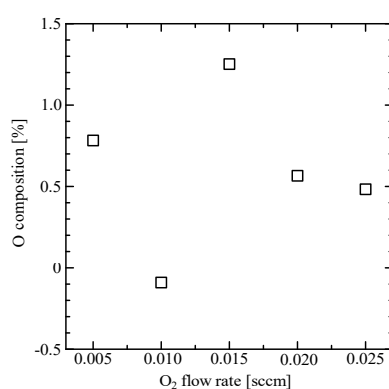


Fig. 2 Relationship between O composition and O₂ flow rate.

[1] K. M. Yu, *et al.*, Phys. Rev. Lett. **91**, 246403 (2003)