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Abstract

This paper provides the correlation between the composition of a given thin film to its optical dispersion properties. Gladstone-Dale (G-D) relationships have been used in optical mineralogy to relate density of crystalline compounds to their average refractive index. We purport to use a 'reverse' G-D approach and determine the composition of multi-component thin films from their optical properties. As a model system, we focus on complex perovskite ferroelectric thin film and apply the derived relationships to determine the stoichiometry. The wavelength dispersion of refractive index and extinction coefficient of various Pb(Zr,Ti)O3 (PZT) thin films was measured using Variable Angle Spectroscopic Ellipsometry. Elemental compositions were measured using Energy Dispersive X-ray analysis and Electron Probe Micro Analysis. Wemple-DiDomenico, Jackson-Amer, Tauc and Urbach optical relationships and related parameters were used to extract correlations to elemental content. Both theoretical and semi-empirical approaches to calculate the electronic polarizability of PZT were employed and their variation with elemental content was computed. Perovskite tolerance and octahedral factors were also analyzed against the optical and polarizability parameters. Lastly, these factors and relationships were combined to realize a model for predicting the elemental content of a thin film system.

Keywords: Thin films; Optical properties; Refractive index; Optical dispersion; Absorption coefficient