T1-P010

Ellipsometric study of Mn-doped Bi₄Ti₃O₁₂ thin films

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Bi₄Ti₃O₁₂ (B₄T₃) is a unique ferroelectric material that has a relatively high dielectric constant, high Curie temperature, high breakdown strength, and large spontaneous polarization. As a result this material has been widely studied for many applications, including nonvolatile ferroelectric random memories, microelectronic mechanical systems, and nonlinear-optical devices. Several reports have appeared on the use of Mn dopants to improve the electrical properties of B₄T₃ thin films. Mn ions have frequently been used for this purpose in thin films and multilayer capacitors in situations where intrinsic oxygen vacancies are the major defects. However, no systematic study of the optical properties of B_4T_3 films has appeared to date. Here, we report optical data for these films, determined by spectroscopic ellipsometry (SE). We also report the effects of thermal annealing and Mn doping on the optical properties. The SE data were analyzed using a multilayer model that is consistent with the original sample structure, specifically surface roughness/B₄T₃ film/Pt/Ti/SiO₂/c-Si). The data are well described by the Tauc-Lorentz dispersion function, which can therefore be used to model the optical properties of these materials. Parameters for reconstructing the dielectric functions of these films are also reported. The SE data show that thermal annealing crystallizes B4T3 films, as confirmed by the appearance of B_4T_3 peaks in X-ray diffraction patterns. The bandgap of B_4T_3 red-shifts with increasing Mn concentration. We interpret this as evidence of the existence deep levels generated by the Mn transition-metal d states. These results will be useful in a number of contexts, including more detailed studies of the optical properties of these materials for engineering high-speed devices.