Temperature-dependent x-ray diffraction of single-crystal, epitaxial films

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The recent availability of commercially-developed, non-ambient stages for measuring epitaxial films with x-ray diffraction now enables routine temperature-dependent measurement of several semiconductor thin-films not otherwise available in bulk form or as powders. To demonstrate the strain evolution and thermal properties of epitaxial films at different temperatures, we use an Anton-Paar DCS 350 stage on a PAN'alytical Empyrean diffractometer to measure antimonide-based strained-layer superlattices (SLS) and epitaxially stabilized α-$Sn_{1-x}Ge_x$ films.

For SLSs we discuss methods for modeling strain in multilayer films under temperature changes whose composite diffraction patterns qualitatively behave differently than those for single-layer films. The modeled diffraction pattern evolves in a predictable fashion as the substrate and layers thermally expand or contract. This modeling includes the estimation of the lattice parameters, coefficients of thermal expansion, and elastic properties of ternary compounds that may not be experimentally known and remains a chief limitation in creating accurate structural models.

We also investigate films that are difficult or impossible to produce in bulk or powder form. In particular, we measure some thermal properties of single-crystal α-$Sn_{1-x}Ge_x$ films. In bulk form, Sn and Ge are practically insoluble (<1 at%), and Sn undergoes the α → β phase transition at 13°C. Despite these apparent limitations on film stability, we produce films with up to 6% Ge compositions and phase stability over 100°C by pseudomorphically growing these alloys on nearly lattice-matched substrates of CdTe and InSb. We exploit our ability to grow these films on two different substrates with sufficiently different coefficients of thermal expansion to determine the relaxed lattice constants, thermal expansion coefficients, and biaxial relaxation constants.

We address basic challenges in calibrating a non-ambient stage without established standards and make recommendations for standards based on our methodology.