Effect of substrate on the atomic structure and physical properties of thermoelectric Ca3Co4O9 thin films.

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While the thermolectric effect has been known for decades, a resurgence of interest in thermoelectrics began in the mid-1990s when theoretical predictions suggested that thermoelectric efficiency could be greatly enhanced through nano-structural engineering, which led to experimental efforts demonstrating proof-of-principle high-efficiency materials [1,2]. In 2001, a benchmark study using nano-structured Bi2Te3–Bi2Se3 superlattices showed a TE figure of merit (ZT) of approximately 2.4 at room temperature, thereby breaking the threshold for efficiently producing electricity using TE devices [3]. The incommensurately layered cobalt oxide Ca3Co4O9 exhibits an unusually high Seebeck coefficient as a polycrystalline bulk material, making it ideally suited for many high temperature thermoelectric applications. In this work, we investigate properties of Ca3Co4O9 thin films grown on cubic perovskite SrTiO3, LaAlO3, and *(*La0.3Sr0.7*)(*Al0.65Ta0.35*)*O3 substrates and on hexagonal Al2O3 (sapphire) substrates using the pulsed laser deposition technique. X-ray diffraction and transmission electron microscopy analysis indicate strain-free growth of films, irrespective of the substrate. However, depending on the lattice and symmetry mismatch, defect-free growth of the hexagonal CoO2 layer is stabilized only after a critical thickness and, in general, we observe the formation of a stable Ca2CoO3 buffer layer near the substrate–film interface. Beyond this critical thickness, a large concentration of CoO2 stacking faults is observed, possibly due to weak interlayer interaction in this layered material. We propose that these stacking faults have a significant impact on the Seebeck coefficient and we report higher values in thinner Ca3Co4O9 films due to additional phonon scattering sites,necessary for improved thermoelectric properties [4].

References

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