

Strategic Superposition: Sb₂Te₃/TiTe₂ Superlattices Possess a Low Thermal Conductivity Contrast, Ideal for PCM

Sepe Van Dyck^{a,*}, Kiumars Aryana^b, Md. Rafiqul Islam^b, William Riffe^b, Patrick Hopkins^b,
Christophe Detavernier^a

^a Dept. of Solid-state Science, Ghent University, Ghent, 9000, Belgium

^b Dept. of Aerospace Engineering, Univ. of Virginia, Charlottesville, VA 22904-4746, USA

Introduction

Reducing the energy consumption of phase change memory (PCM) is one of the biggest hurdles towards its implementation. The switching mechanism in PCM consists of applying enough heat to the material to change it from crystalline to amorphous or vice versa. Diffusion of this heat into the surroundings of the cell is therefore detrimental. The thermal conductivity of the phase change material and its surroundings plays a crucial role in reducing the energy needed for a PCM to function. A good PCM material should have low thermal conductivity in both its crystalline and amorphous phase. Typical materials such as GST on the other hand, display a significant contrast in their thermal conductivity [2]. As a possible improvement we study Sb₂Te₃/TiTe₂ superlattices, a material system first proposed by Shen et al. in reference [1] showing a significant reduction in its reset power consumption. After deposition and structural characterization of these superlattices, the thermal transport properties are examined using time-domain thermoreflectance (TDTR).

Methods

All samples are created through magnetron co-sputtering from elementary pure targets in a variation of the modulated reactants method [3]. This method has been shown to create high-quality and planarly texturized layers with the 00L family of planes parallel to the substrate upon crystallization. This is verified through *in situ* and *ex situ* XRD and rocking curve analysis. Time-domain thermoreflectance (TDTR) measurements are performed in a two-tint setup. This a laser pump-probe technique with which the cross-plane thermal conductivity of thin films can be accurately measured. These measurements are performed at room temperature for different thicknesses and at increased temperatures under an inert atmosphere to study the evolution of the thermal conductivity upon crystallization.

Structural Characterization

XRD patterns for films of the individual materials as well as their superlattice can be seen in figure 1. The intensity and presence of the 00L peaks are indicative of a strong crystalline texture of the films. The evolution of an as-deposited superlattice upon anneal is visible in figure 2. Crystallization and melting of Sb₂Te₃ are visible. The intense satellite peaks are indicative of the layered structure [4].

Thermal Conductivity Results

TDTR results of single-layer samples of the individual materials are shown in figure 3. Both materials show a relatively low thermal conductivity in their as-deposited state, while (further) crystallization upon anneal increases it. The *in situ* data for a single 80nm Sb₂Te₃ layer can be seen in figure 4 where it is presented next to data for 16-period thick superlattices. A set of three types of superlattice is studied: 5nm of Sb₂Te₃ is combined with either 3nm, 6nm or 9nm TiTe₂. At room temperature we see that the relative composition has little effect on the as-deposited samples. This can be explained by the high thermal resistance of the amorphous Sb₂Te₃ sub-layers that dominate the stack. During anneal the thermal conductivity of all superlattices increases. Although upon cooling down, the value for the 5-3 superlattice drops down to the same value as before the anneal, reducing all contrast in thermal conductivity between the crystalline and amorphous phase.

Conclusions

The superlattice consisting of 5nm Sb₂Te₃ and 3nm TiTe₂ shows a minimal contrast in thermal conductivity between its two phases at room temperature, making it better suited than a single layer of Sb₂Te₃ for use as a phase change material. All superlattices demonstrate a lower thermal conductivity than the bulk as well as a decreased contrast. This might indicate that the superlattice's added interfaces not only introduce a thermal resistance, but also influence the phononic landscape, leading to the low thermal conductivity contrast that is observed.

References

1. K. Aryana *et al.*, Nat. Commun. **12**, 774 (2021).
2. M. Noh *et al.*, Science **270**, 1181 (1995).
3. J. Shen *et al.*, ACS Appl. Mater. Interfaces **11**, 5336 (2019).
4. R. Venkatasubramanian *et al.*, J. Cryst. Growth **170**, 817 (1997).

* corresponding author e-mail: Sepe.VanDyck@UGent.be

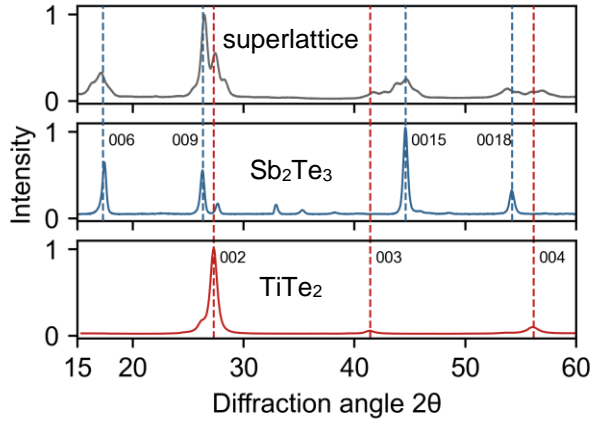


Fig. 1: The XRD pattern of an annealed superlattice shows peaks of both bulk Sb_2Te_3 and TiTe_2 . The presence of satellite peaks is indicative of the superlattice structure.

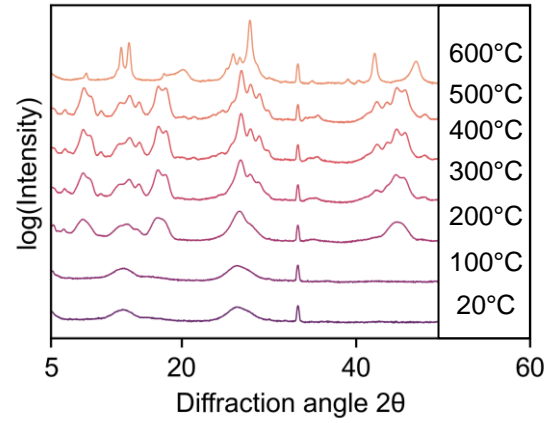


Fig. 2: *Ex situ* scans of a superlattice annealed at different temperatures show the crystallization and subsequent melting of Sb_2Te_3 .

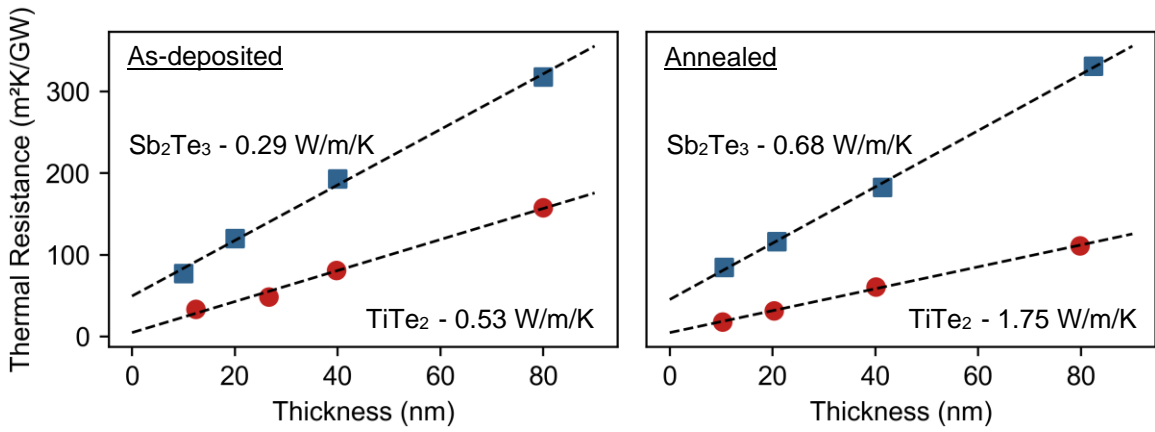


Fig. 3: The intrinsic thermal conductivity of the single layer materials is calculated by combining results for several thicknesses and performing a linear fit. These results show the thermal conductivity contrast between as-deposited samples and after a 300°C ramp anneal.

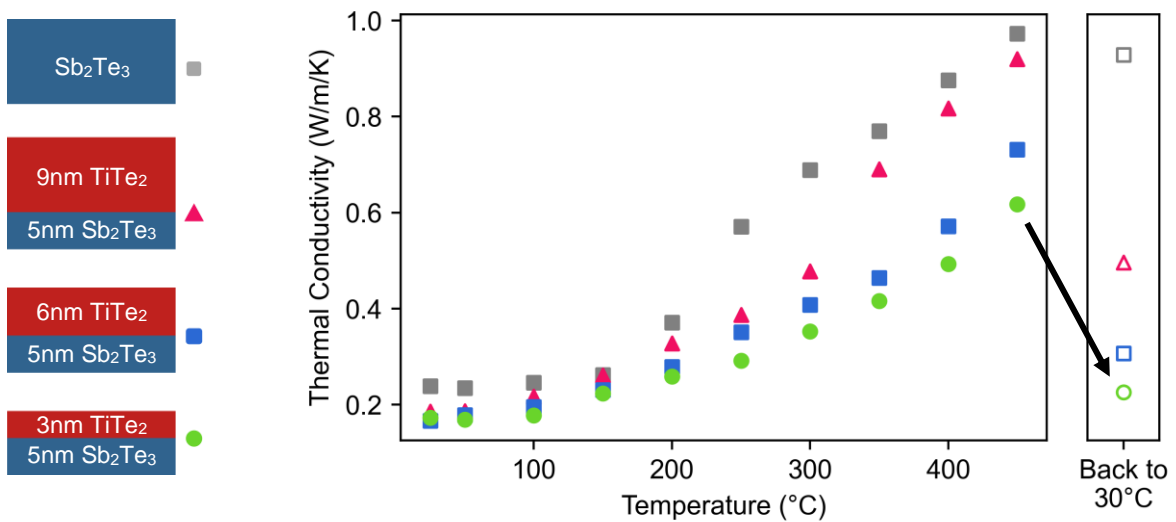


Fig. 4: Three types of superlattices are compared to bulk Sb_2Te_3 during *in situ* TDTR measurements. Thermal conductivity increases for all samples when heating up. After cooling down the 5-3 superlattice still shows a very low thermal conductivity, despite its crystallinity.