Picking the Right TMD is the Key to Controlling Heat In a Phase Change Superlattice

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Introduction

Although phase change materials, such as GST, generally boast a low thermal conductivity in the amorphous phase, this often changes drastically upon crystallization. This is problematic as a loss of energy, due to heat diffusion into the surroundings, contributes to the high energy consumption of this novel type of memory. One promising way of tackling this high contrast in thermal conductivity, is by incorporating the phase change material into a superlattice. For example, interlacing Sb_2Te_3 with thin layers of $TiTe_2$ has proven to reduce the thermal conductivity, even in the crystalline phase. This in turn contributes to the superb performance, demonstrated by these structures [1]. TiTe2 has, by itself, a relatively high thermal conductivity, which begs the question if TiTe2 is the best choice for this application. In the search for new materials to be used in these superlattices, three alternative transition-metal ditellurides are presented: WTe_2, VTe_2 and $ZrTe_2$.

Methods

To create the different metal-ditelluride films and superlattices, magnetron sputtering is applied from elementary pure targets. Magnetrons are energized in a planetary geometry, while the substrate passes underneath. Through this way, the stoichiometry of the deposited layer can be controlled and highly crystalline materials can be achieved after anneal [2]. An automated shutter system is used to create the superlattice of Sb_2Te_3 and the different MTe_2 candidates. Thermal conductivity is measured using time-domain thermoreflectance (TDTR), a laser-based pump probe technique that can directly probes the thermal response of a system of thin-films. Samples are covered with a 80nm Ru transducer. The transducer turns the power of the laser into heat (pump), while its reflectivity acts as an indicator of the surface temperature (probe) [3].

Structural Characterization

The three materials show little to no crystallinity right after deposition. While both VTe_2 and $ZrTe_2$ crystallize upon anneal, we were not able to crystallize WTe_2. For this reason, we focus solely on the first two materials. After an anneal to 300°C, both materials crystallize into a highly textured CdI_2 structure with 00L planes parallel to the Si substrate. This can be seen in the rocking curve and XRD data shown in Fig. 1. A sample containing 80nm VTe_2 is shown on the left, the right side shows a 5nm Sb_2Te_3 / 3nm $ZrTe_2$ superlattice. Peaks of both materials are present in the superlattice, next to satellite peaks that are a result of the superlattice structure.

Thermal Conductivity Results

A room-temperature study of all three candidate materials is first performed. Creating a thickness series allows us to extrapolate-out interface resistances and reveal the intrinsic thermal conductivity of the materials. An example of this analysis for $ZrTe_2$ is shown on the left of Fig. 2. On the right, a comparison is made between the three candidate materials, $TiTe_2$ and Sb_2Te_3. All three candidates have very little contrast between the two states, with $ZrTe_2$ displaying the lowest thermal conductivity. To characterize $ZrTe_2$ even further, an in situ study is performed, results can be seen in Fig. 3. After crystallization, the thermal conductivity for $ZrTe_2$ stays under that of Sb_2Te_3, which is exactly what is wanted for a good superlattice. A 5nm Sb_2Te_3 / 3nm $ZrTe_2$ superlattice displays a consistently low thermal conductivity all the way up to 450°C..

Conclusions

Both VTe_2 and $ZrTe_2$ make promising candidates for use in PCM superlattices due to their high crystalline quality, thermal stability and consistently low thermal conductivity contrast. On top of this, $ZrTe_2$ and its superlattice demonstrate a low thermal conductivity, even at high temperatures, making it a prime candidate for further investigations.

References

1. K. Ding et al., Science **366**, 210 (2019)
2. M. Noh et al., Science **270**, 1181 (1995)
3. D. G. Cahill, Rev. Sci. Instrum. **75**, 12 (2004)

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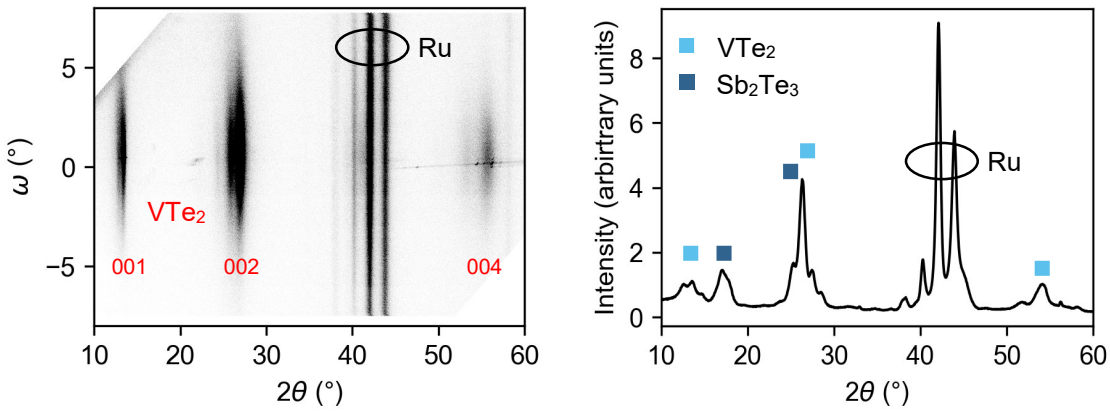

Figure 1. (left) XRD and rocking curve data show the high quality and structure of sputtered VTe_2 after an anneal to 450°C. The 80nm ruthenium transducer layer is also visible. **(right)** XRD data for the VTe_2 /Sb_2Te_3 superlattice shows that both phases are present in the superlattice. The visible satellite peaks indicate an ordered superlattice structure.

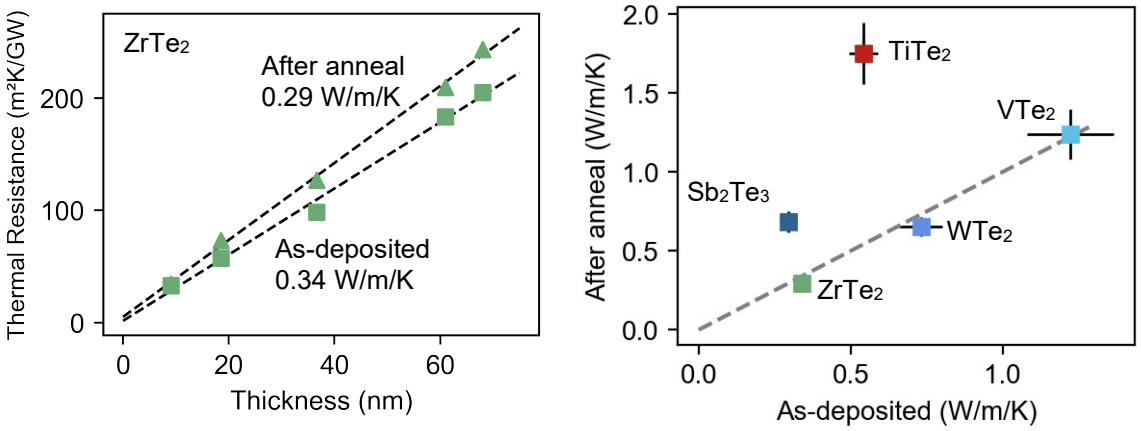

Figure 2. (left) Creating a thickness series of the same material, allows us to calculate the intrinsic thermal conductivity of the materials. Shown is the data for $ZrTe_2$ between 10 and 80 nm. **(right)** All three materials show a very low contrast in thermal conductivity. They lie close to dashed line, which signifies zero contrast.

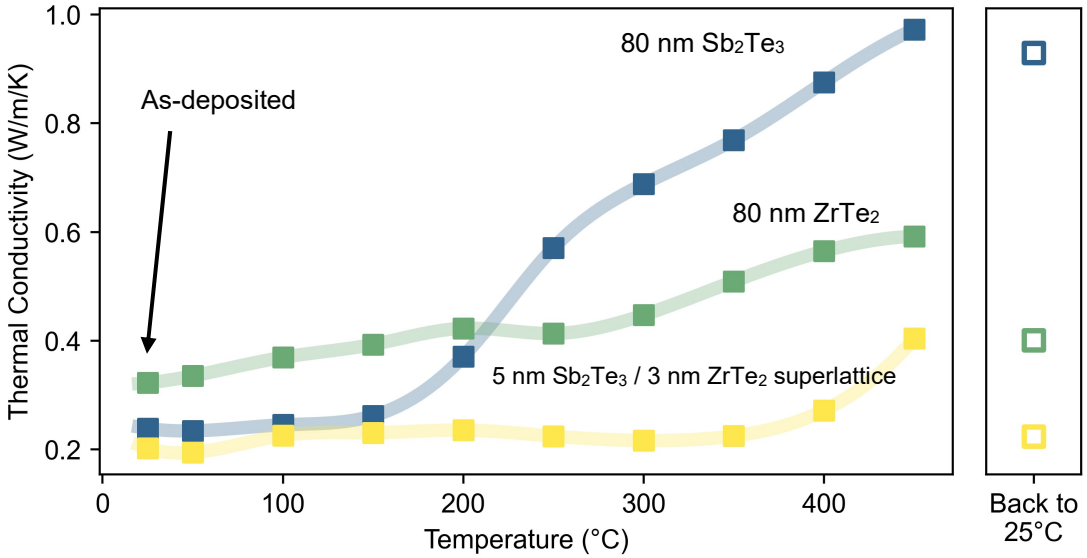

Figure 5 At high temperatures the thermal conductivity of $ZrTe_2$ only increases slightly, while that of Sb_2Te_3 increases drastically. The superlattice with 16 periods of these materials performs very well in the studied temperature range.