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HEAT CONDUCTION ACROSS NANOSCALE INTERFACES AND NANOMATERIALS FOR THERMAL MANAGEMENT AND THERMOELECTRIC ENERGY CONVERSION

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ABSTRACT

Nanoscale heat conduction plays a critical role in applications ranging from thermal management of nanodevices to nanostructured thermoelectric materials for solid state refrigeration and power generation. This lecture presents recent investigations in our group. The first part of the lecture demonstrates heat conduction across nanoscale interfaces formed between individual nanoscale heaters and the silicon substrate [1]. A systematic experimental study was performed of thermal transport from individual nanoscale heaters with widths ranging between 77nm-250nm to bulk silicon substrates in the temperature range of 80-300K. The effective substrate thermal conductivity was measured by joule heating thermometry. We report up to two orders of magnitude reductions in the measured effective thermal conductivity of the silicon substrate when the heater widths are smaller than the mean free path of the heat carriers in the substrate, as summarized in Fig. 1. The effective mean free path of the silicon substrate was extracted from the measurements and was found to be comparable with recent molecular dynamics simulations.

A proof of concept demonstration of a novel Thermal Interface Material (TIM) is presented next. The high thermal conductivity TIM is based on a highly connected high thermal conductivity nanostructured filler network embedded in a polymer matrix where the contribution of filler-matrix interfaces to thermal resistance is minimized. It was found [2] that the thermal conductivity could be varied from ~0.2 to 20 W/mK when the volume fraction of metallic nanoparticles was varied from 0 – 20%. For similar volume fractions and filler composition, microparticle based composites have two orders of magnitude lower thermal conductivities. SEM characterization and thermal transport modeling are employed to support the conclusion that morphological changes in the nano-TIM are responsible for the thermal conductivity reduction.

Thermoelectric transport investigations are discussed for a novel class of highly scalable nanostructured bulk chalcogenides developed at Rensselaer Polytechnic Institute [3]. Un-optimized, single-component bulk assemblies of Bi_2Te_3 and Sb_2Te_3 single crystal nanoplates show large enhancements (25-60%) in the room temperature thermoelectric figure of merit compared with individual bulk counterparts (Table 1). Nanostructuring was found to lead to strong thermal conductivity reduction without significantly affecting the mobility of the charge carriers, as shown in Table 2.

A scanning thermal microprobe technique developed for simultaneous thermal conductivity (κ) and Seebeck coefficient (α) measurements in thermoelectric films is also presented [4].

In this technique, an AC alternative current joule-heated V-shaped microwire that serves as heater, thermometer and

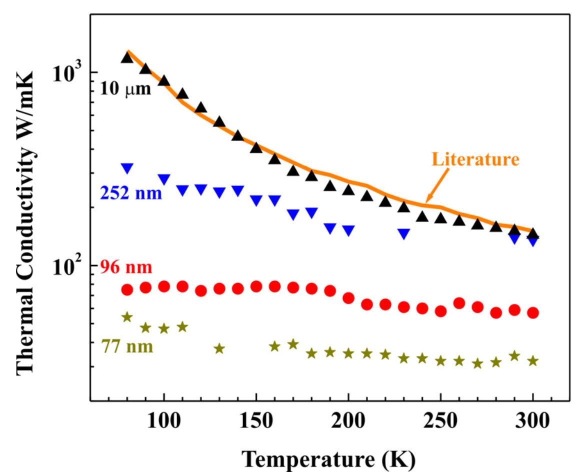

Fig. 1 Temperature dependent effective thermal conductivity of silicon substrates as measured by heater wires of widths 10 µm, 252 nm, 96 nm and 77 nm in the temperature range 300 - 80 K [1]. The reported literature value of the thermal conductivity of silicon is plotted for comparison. Up to two orders of magnitude reduction in the effective substrate thermal conductivity occurs due to the size-effect of nanoscale heat source.

voltage electrode, locally heats the thin film when contacted with the surface (Fig. 2). The κ is extracted from the average DC temperature rise thermal resistance of the microprobe and α from the DC Seebeck voltage measured between the probe and unheated regions of the film by modeling the heat transfer in the probe, sample and their contact area, and by calibrations with standard reference samples. Application of the technique on sulfur-doped porous Bi_2Te_3 and Bi_2Se_3 films reveals α= -105.4 and 1.96 μV/K, respectively, which are within 2% of the values obtained by independent measurements carried out using microfabricated test structures. The respective κ values are 0.36 and 0.52 W/mK, which are significantly lower than the bulk values due to film porosity, and are consistent with effective media theory. The dominance of air conduction at the probe-sample contact area determines the microscale spatial resolution of the technique and allows probing samples with rough surfaces. Non-contact mode measurement of thermal conductivity was also demonstrated and confirmed by independent characterization [5]. In non-contact mode the technique utilizes ballistic air conduction as the dominant heat transfer mechanism between the thermal probe and the sample and thus eliminates uncertainties due to solid contact and liquid meniscus conduction.

Table 1 Summary of thermoelectric properties at 300K for selected nanostructured bulk chalcogenides with enhanced figure of merit ZT.

	σ 10^5 S/m	α μV/K	κ W/mK	$κ_L$ W/mK	ZT 300 K
Bi_2Te_3	1.3	-185	1.23	0.54	1.1
Bi_2Se_3	0.77	-82	0.7	------	0.22
Sb_2Te_3	1.2	133	0.8	------	0.74
$(BiSb)_2Te_3$	0.17	285	0.39	0.3	1.05

Table 2 Mobility and charge carrier concentrations of selected single component nanostructured bulk materials compared to the single crystal bulk literature values along different directions.

		σ (10^5S/m)	Carrier Concentration(cm^{-3})	Mobility (cm^2/Vs)
Nano-Bi_2Te_3		1.7	$6.9×10^{19}$	150
Nano-Sb_2Te_3		1.06	$3.7×10^{19}$	180
Bi_2Te_3 (CRC)	11	2.2	$5.2×10^{19}$	171
	33	0.42	$5.2×10^{19}$	50
Sb_2Te_3 (CRC)	33	1.93	$1.65×10^{20}$	73
	11	6.9	$1.65×10^{20}$	262

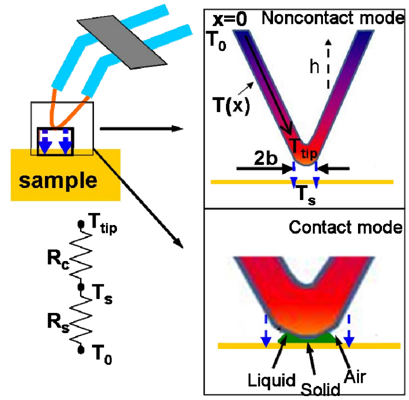

Fig. 2 The principle underpinning the scanning thermal microprobe technique. The microprobe serves as both a heater and a thermometer when electrical current is passed through it. In contact mode simultaneous Seebeck and thermal conductivity measurements are performed. For non-contact thermal conductivity measurements, the microprobe is brought in the proximity of the sample, to ~100 nm above the sample surface were ballistic air conduction is employed as the major mechanisms for tip-sample heat transfer.

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