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In 2014 Zhao *et al*. [1] at Northwestern University reported that they have found an ultralow thermal conductivity (<0.4$Wm^{-1}K^{-1}$ at 923 K) and high thermoelectric figure of merit (*ZT*~2.6±0.3 at 923 K) in SnSe crystals, and have the results published in **Nature** (17 April VOL 508, Nature 375). Indeed, it is a breaking news to the world because the *ZT*~2.6±0.3 (represents thermoelectric performance) is a world record for the thermoelectric materials (ZT=2.4 for super lattice Bi_2Te_3-Sb_2Te_3) ever found, especially for the pure bulk crystal (maximum ZT=1). The *ZT*~2.6 stands for that the material is an excellent green energy thermoelectric material and has the capability of transfer heat to electricity with efficiency >20% which almost compete with the best solar cell nowadays. Unfortunately, no any group can reproduce the record high figure of merit *ZT* of SnSe.

The material is shortly studied by the Dr. Chen group in the institute of physics, Academia Sinica, they found the maximum ZT~1, then Dr. Rao group in Clemson joins the study. After carefully compare the data of our and those of Zhao *et al*, we deduce that their samples are not fully dense (5.4 g/cm^3 which is only 87% of the theoretical value 6.2 g/cm^3) and thus not truly single crystalline, implying that their reported thermal conductivities are not intrinsic to SnSe. After found the discrepancy of their SnSe crystal is not true single crystal of SnSe, we raised the issue and prepared a complete evidence and analysis to the Nature, and have our discovery released in the Nature (3 NOVEMBER 2016 VOL 539 NATURE E1).

In this work, we have grown the best SnSe single crystal in the world, and reported the intrinsic thermal conductivity of SnSe. This research work offers a better understanding of the SnSe crystal, and warrants further investigation into intrinsic thermal transport in SnSe single crystals and its use as a thermoelectric material.

1. Zhao et al Nature 508, 373-377 (2014)

熱電材料硒化錫(SnSe)晶體之真實熱傳導係數

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2014 年美國西北大學 Zhao et al 等人於自然期刊發表了硒化錫晶體超低之熱傳導係數 κ (<0.4 $Wm^{-1}K^{-1}$ at 923 K) 與很高的熱電優質參數 (*ZT*~2.6 at 923 K)。此一發現當時震驚了科學界, 因為優質係數 ZT=2.6 是熱電材料的世界紀錄（雖然超晶格 Bi_2Te_3-Sb_2Te_3 ZT=2.4), 但對純塊材而言 ZT=1 就已經很了不起了。 ZT=2.6 意味著此一材料具有極佳之熱電轉換效率 > 20%, 此一效率幾可與目前最好的太陽能電池相比擬。可惜的是世界上一直沒有一個研究團隊有辦法複製此一研究成果。

由中央研究院物理研究所陳洋元博士帶領的研究團隊,隨即長出硒化錫之單晶後, 經過的精密的實驗量測後, 我們發現在 923 K *ZT* 僅有 1 左右, 此時 Dr. Rao 的團隊加入, 我們仔細比對雙方之數據後,發現 Zhao et al 等人的硒化錫之樣品並非真正之單晶, 其密度(5.4 g/cm^3)約只有真正單晶密度(6.2 g/cm^3)的 87%。這說明了西北大學 Zhao et al 等人於自然期刊發表的結果並非真正硒化錫晶體應有之物理特性。發現美國西北大學 Zhao et al 的硒化錫晶體有問題後,我們將此一發現與我們完整之數據提報給 Nature 期刊, 經過專家學者之審查後, 證明 Zhao et al 的結果確實有問題,於是將我們的發現呈現於今年 11 月 3 日的 自然期刊。於此一研究我們長出了世界第一個真正完美的 SnSe 單晶, 也量測出此單晶之本徵熱傳導係數, 對了解目前最熱門之熱電材料-硒化錫之研究做出了重大之貢獻。

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