

ESI for:

Low temperature CVD of thermoelectric SnTe thin films from the single source
precursor [n Bu₃Sn(Te n Bu)]

Fred Robinson, Daniel W. Newbrook, Peter Curran, C. H. (Kees) de Groot, Duncan Hardie, Andrew L. Hector, Ruomeng Huang and Gillian Reid

Contents:

Figure S1 NMR spectra for [n Bu₃Sn(Te n Bu)] in CDCl₃ at 295 K.

Figure S2 Isothermal step TGA experiment of Bu₄Sn used for vapour pressure calculation.

Figure S3 Grazing incidence XRD data for SnTe samples FR148T8 (black), FR148T7 (red), FR146T5 (green), FR173T4 (blue) and ICSD-188457 (bottom red).¹

Table S1 Lattice parameters calculated from decomposition analysis of XRD patterns of thin films of SnTe, crystallite sizes acquired using the Halder-Wagner method and literature values.

Figure S4 Lower magnification SEM images of films deposited by CVD onto fused SiO₂ substrates showing uniform film deposition and the corresponding EDX spectra for; tile (a) deposition 1 tile 2, (b) deposition 2 tile 1, (c) deposition 2 tile 2 and (d) deposition 3 tile 1.

Figure S5 Halder-Wagner plots with trend lines obtained by linear regression analysis.

Figure S1 NMR spectra for $[\text{}^n\text{Bu}_3\text{Sn}(\text{Te}^n\text{Bu})]$ in CDCl_3 at 295 K.

Figure S1.1 The ^1H NMR spectrum.

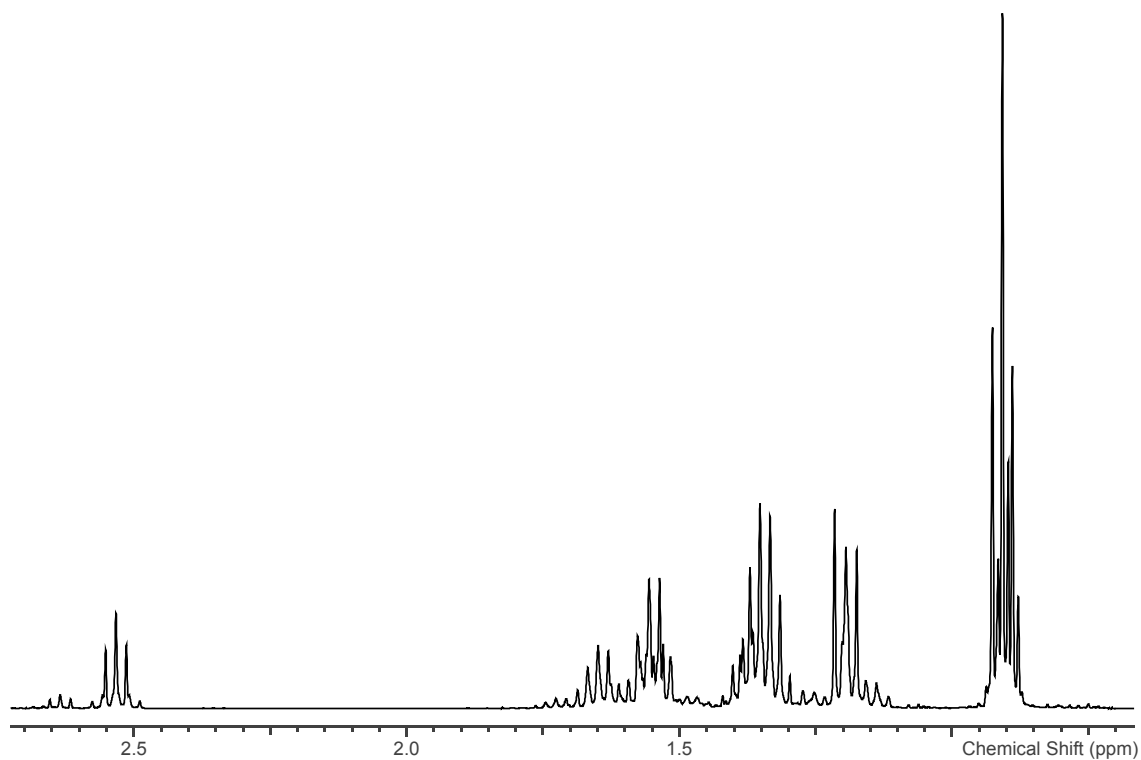


Figure S1.2 The $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum.

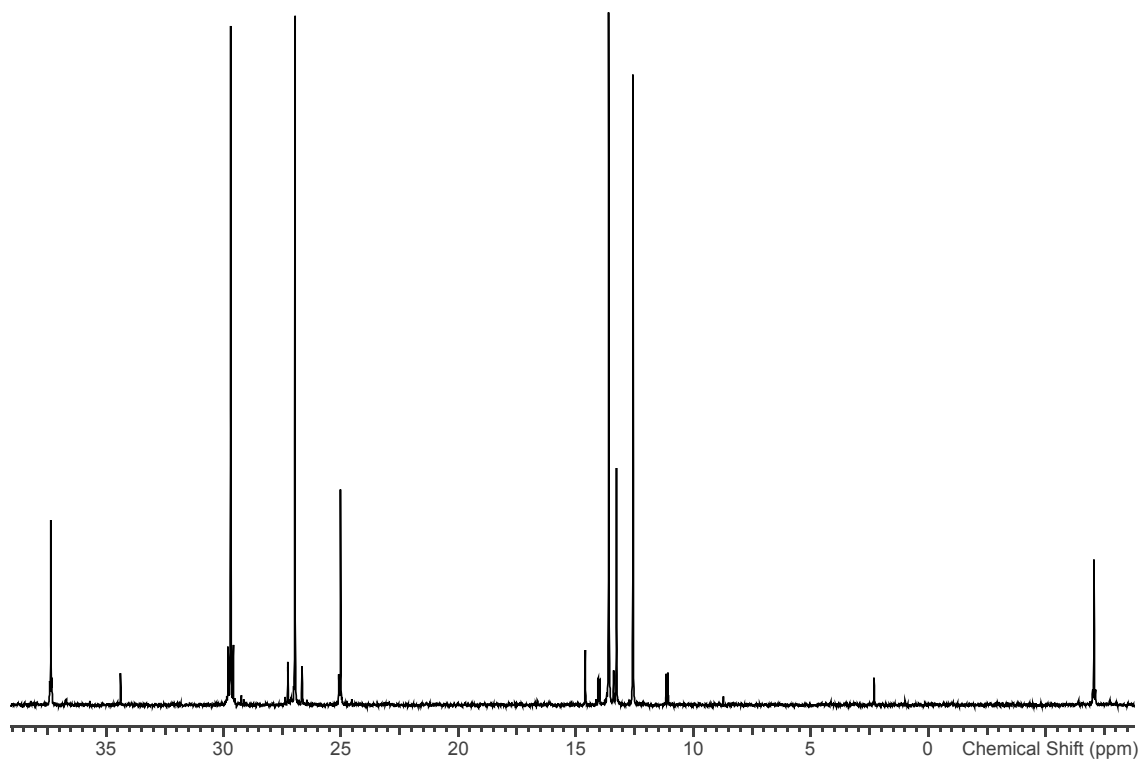


Figure S1.3 The 2D HSQC NMR spectrum.

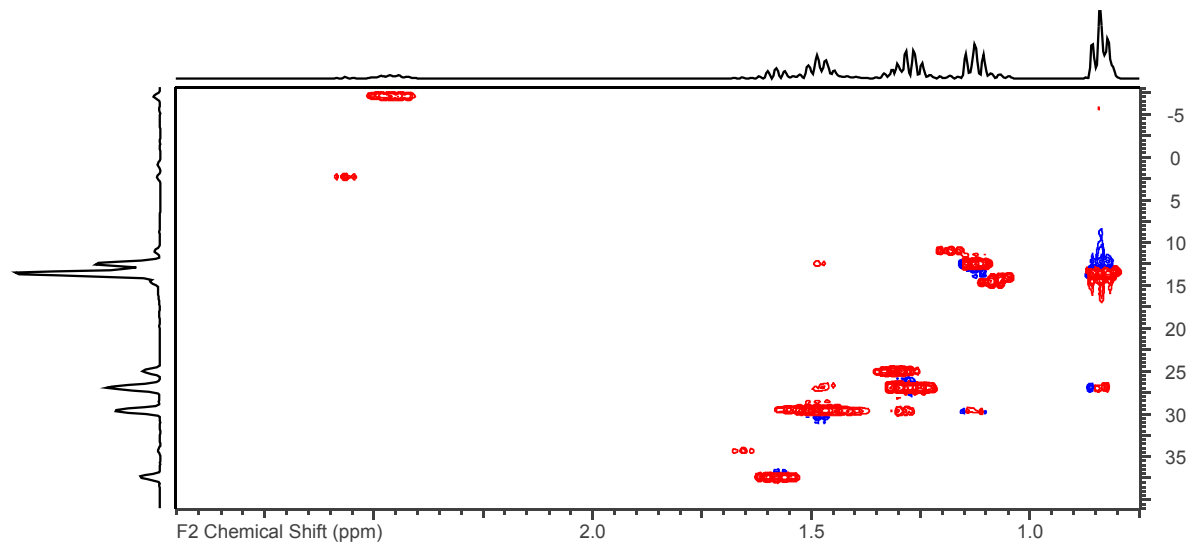


Figure S1.4 The $^{119}\text{Sn}\{^1\text{H}\}$ NMR spectrum.

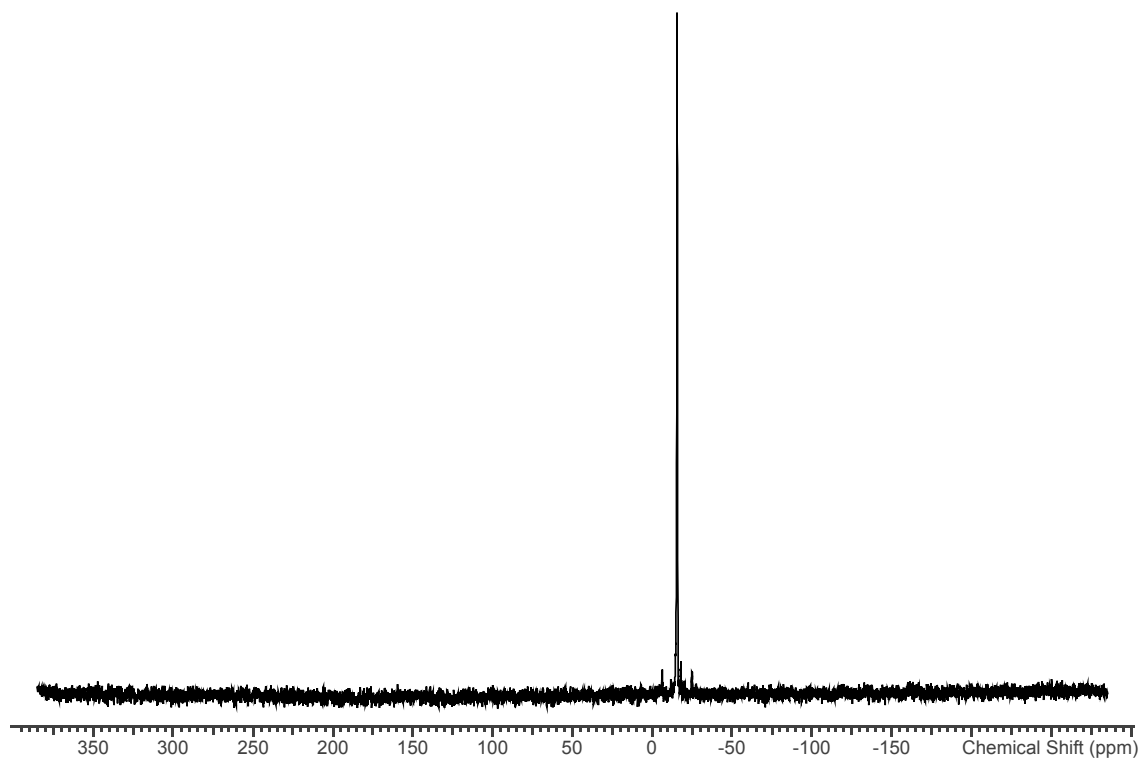


Figure S1.5 The $^{125}\text{Te}\{^1\text{H}\}$ NMR spectrum.

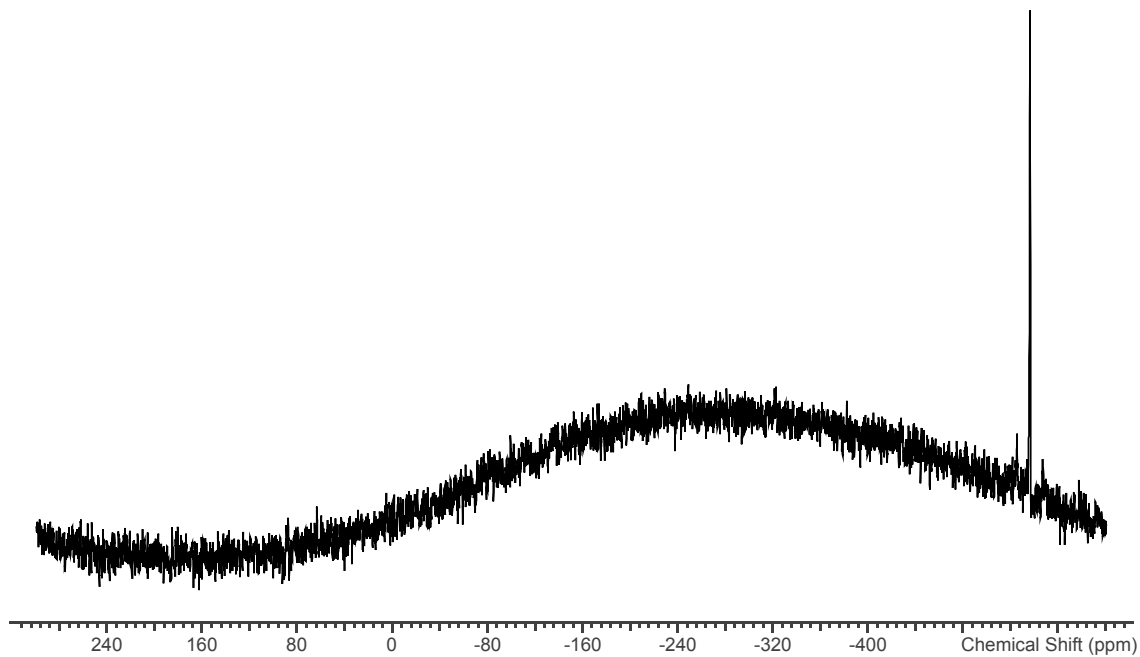


Figure S2 Isothermal step TGA experiment of Bu_4Sn used for vapour pressure calculation.

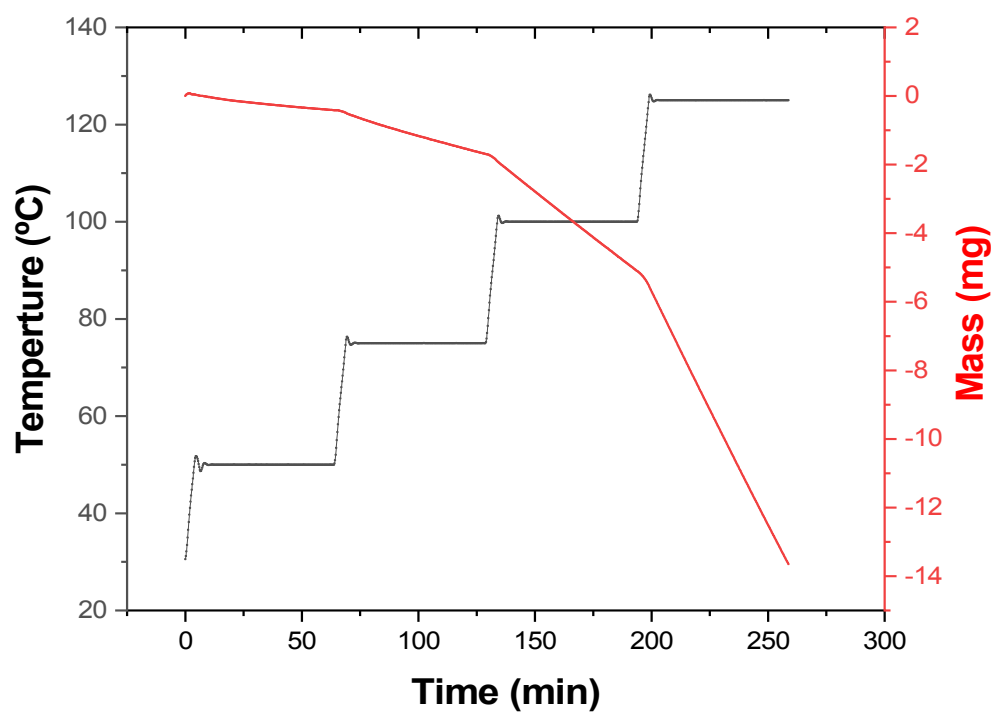


Figure S3 Grazing incidence XRD data for SnTe samples deposition 2 tile 2 (black), deposition 2 tile 1 (green), deposition 1 tile 1 (purple), deposition 3 tile 1 (blue) and ICSD-188457 (bottom red).¹

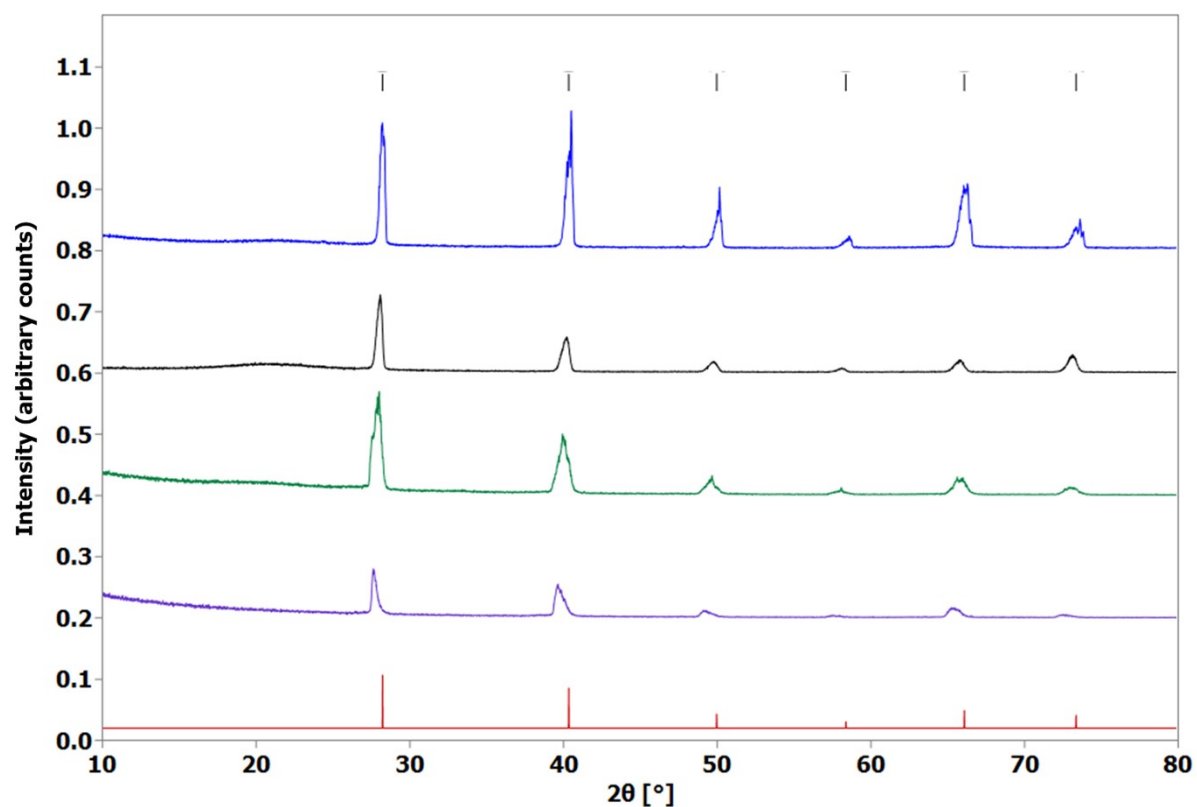
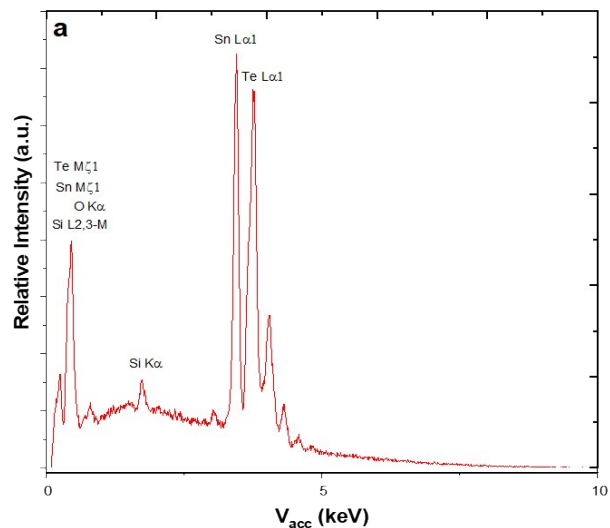
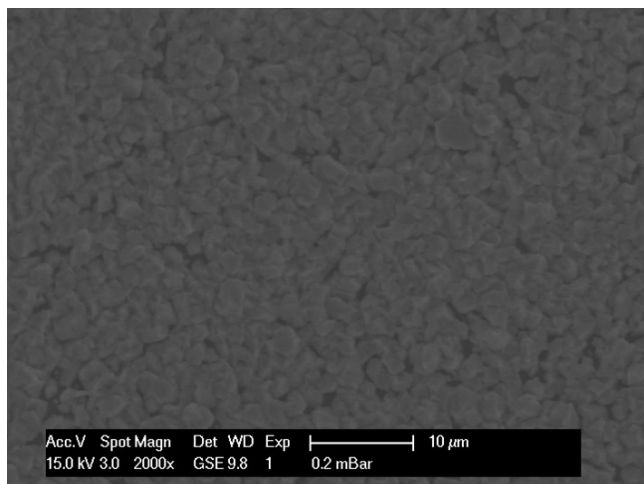


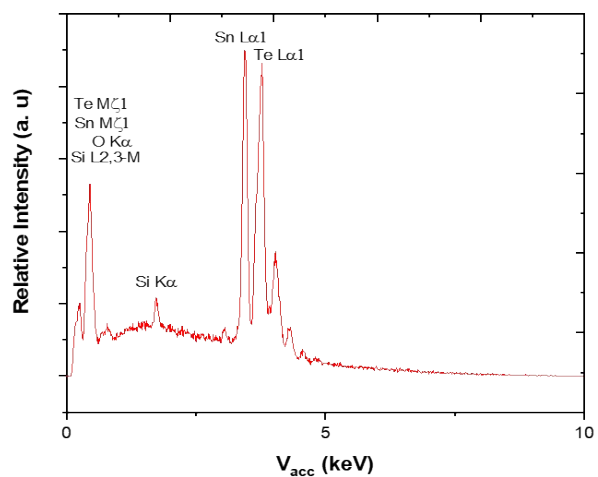
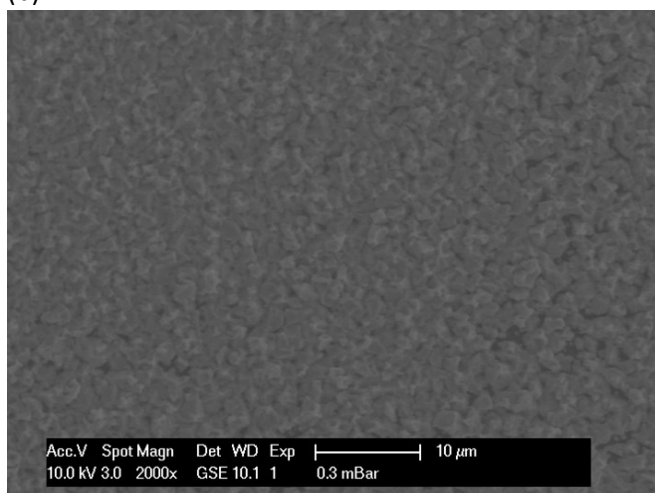
Table S1 Lattice parameters calculated from decomposition analysis of XRD patterns of thin films of SnTe, crystallite sizes acquired using the Halder-Wagner method and literature values. *Lanthanum hexaboride standard used and matched to a literature pattern.²

Data	Deposition Temperature (°C)	a (Å)	R _{wp} %	R _p %	Crystallite size (nm) with standard*
Deposition 1 Tile 1	404	6.3881(3)	14.30	9.82	110(30)
Deposition 2 Tile 1	410	6.35250(18)	15.50	10.82	100(10)
Deposition 2 Tile 2	355	6.3304(4)	12.59	9.29	210(110)
Deposition 3 Tile 1	434	6.30301(19)	12.73	9.75	-
Bulk SnTe ¹	-	6.318(3)	13.70	13.60	-

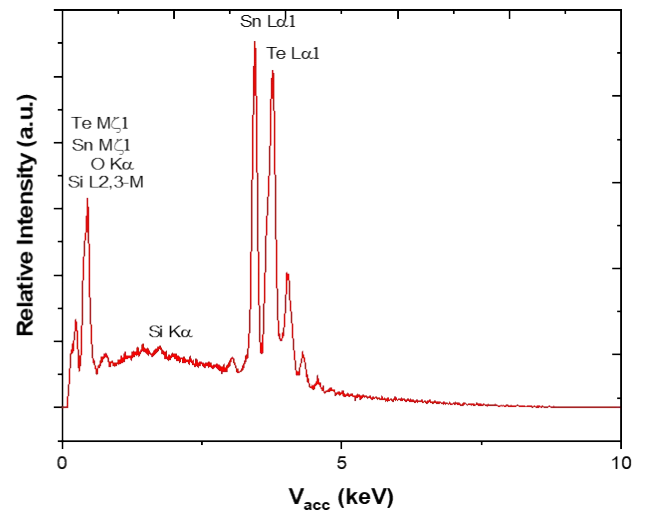
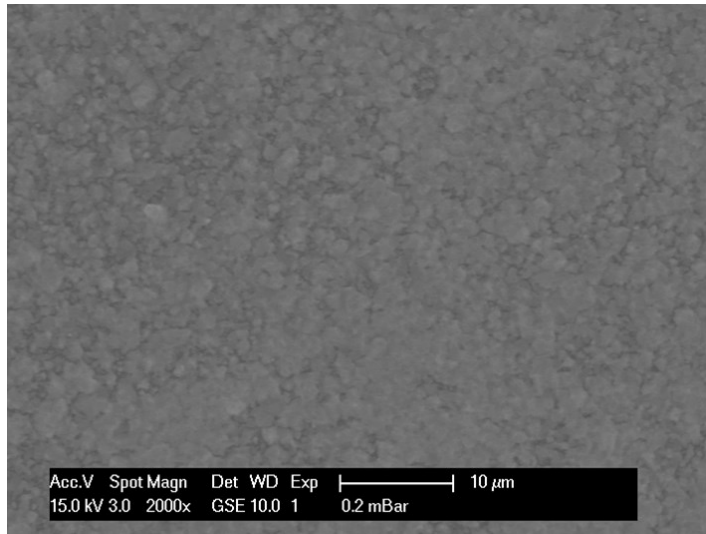
Figure S4 Lower magnification SEM images of films deposited by CVD onto fused SiO₂ substrates showing uniform film deposition and the corresponding EDX spectra for; tile (a) deposition 1 tile 2, (b) deposition 2 tile 1, (c) deposition 2 tile 2 and (d) deposition 3 tile 1.



(b)



(c)



(d)

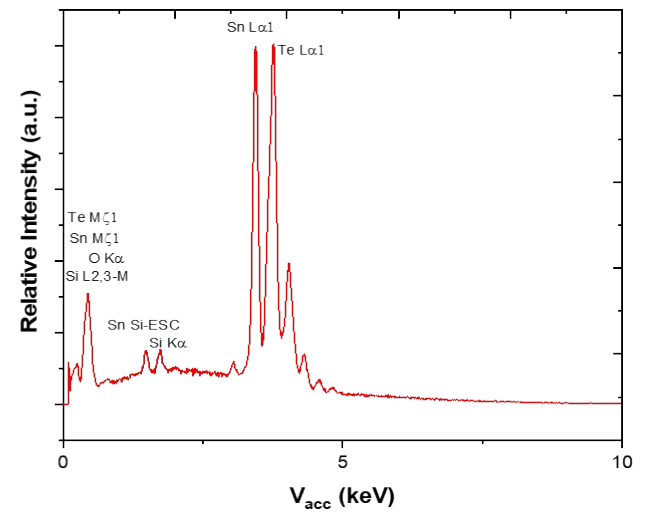
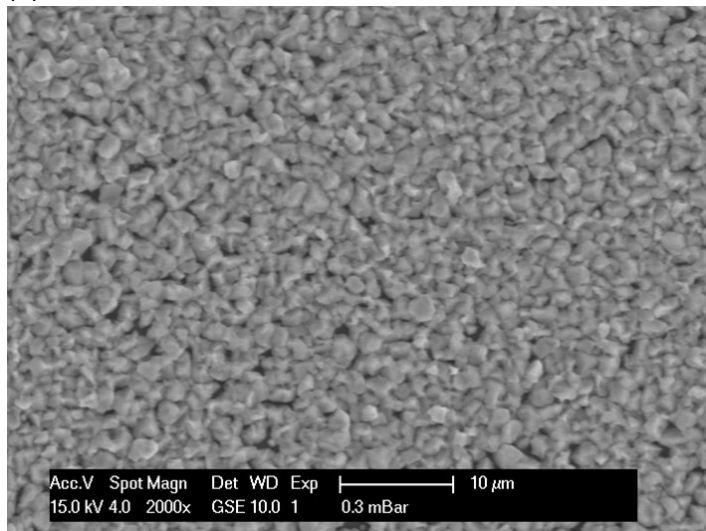


Figure S5 Halder-Wagner plots with trend lines obtained by linear regression analysis and compared to a lanthanum hexaboride standard to account for instrumental peak broadening.

Figure S5.1 Plot for Deposition 1 tile 1.

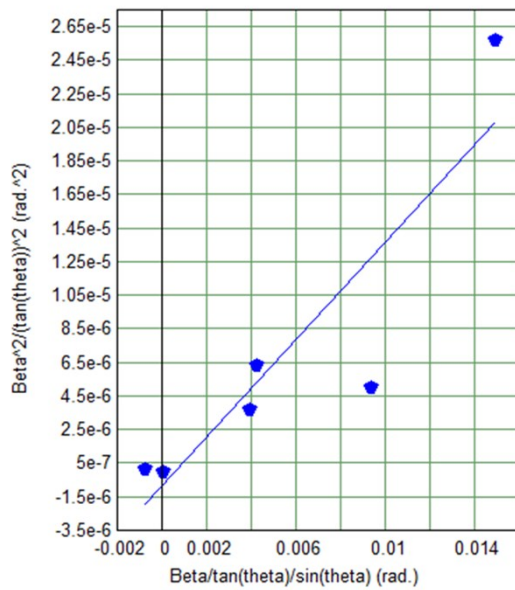


Figure S5.2 Plot for Deposition 2 tile 1.

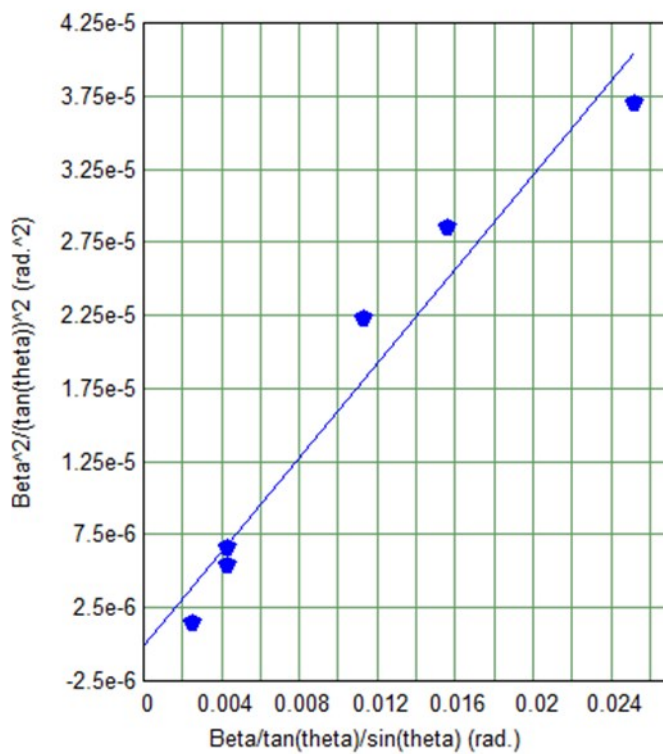


Figure S5.3 Plot for Deposition 2 tile 2.

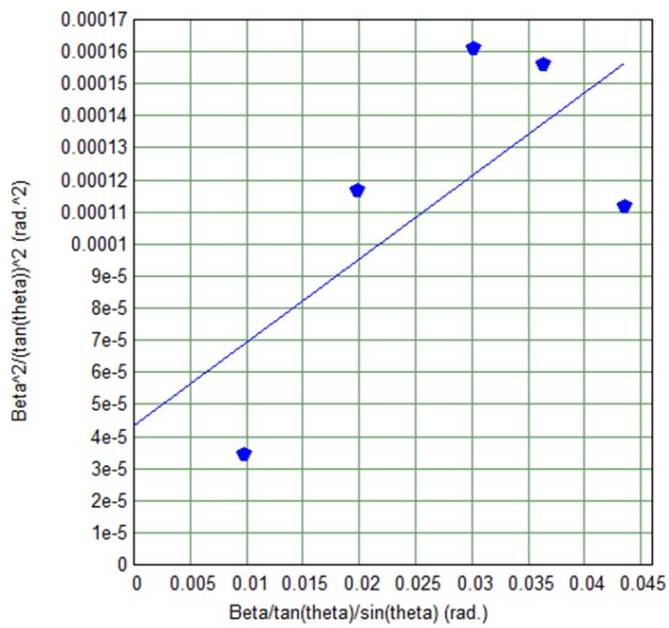
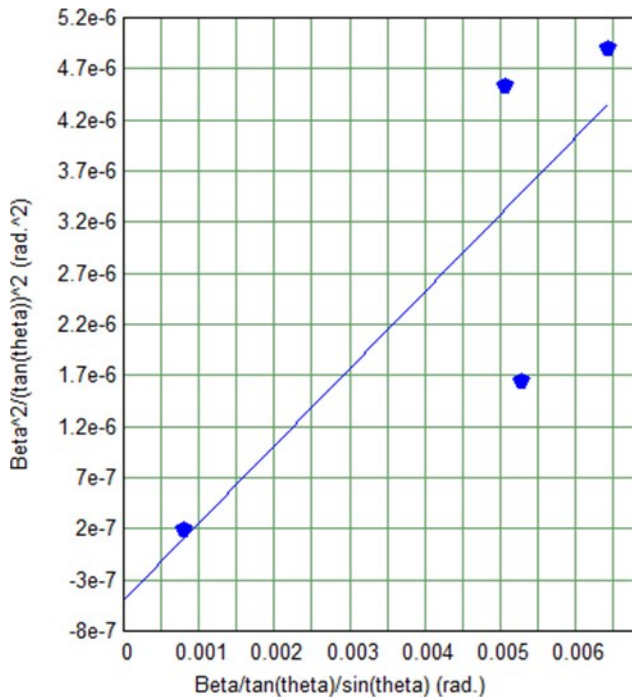


Figure S5.4 Plot for Deposition 3 tile 1.



References

- 1 P. Bauer Pereira, I. Sergueev, S. Gorsse, J. Dadda, E. Müller and R. P. Hermann, *Phys. status. Solidi B*, 2013, **250**, 1300.
- 2 A. A. Eliseev, G. M. Efremmov, V A Kuz'micheva, E. S. Konovalova, V. I. Lazorenko, Y. B. Paderno and S. Y. Khlyustova, *Kristallografiya*, 1986, **31**, 803.