Synthesis, Polymorphism, and Electronic Structures of $Sr_3Sn_2As_4$

Xiao-Cun Liu, Ming-Yan Pan, Xin Li, Sheng-Qing Xia, and Xu-Tang Tao*

State Key Laboratory of Crystal Materials, Institute of Crystal Materials,

Shandong University, Jinan, Shandong 250100, People's Republic of China

Supporting Information

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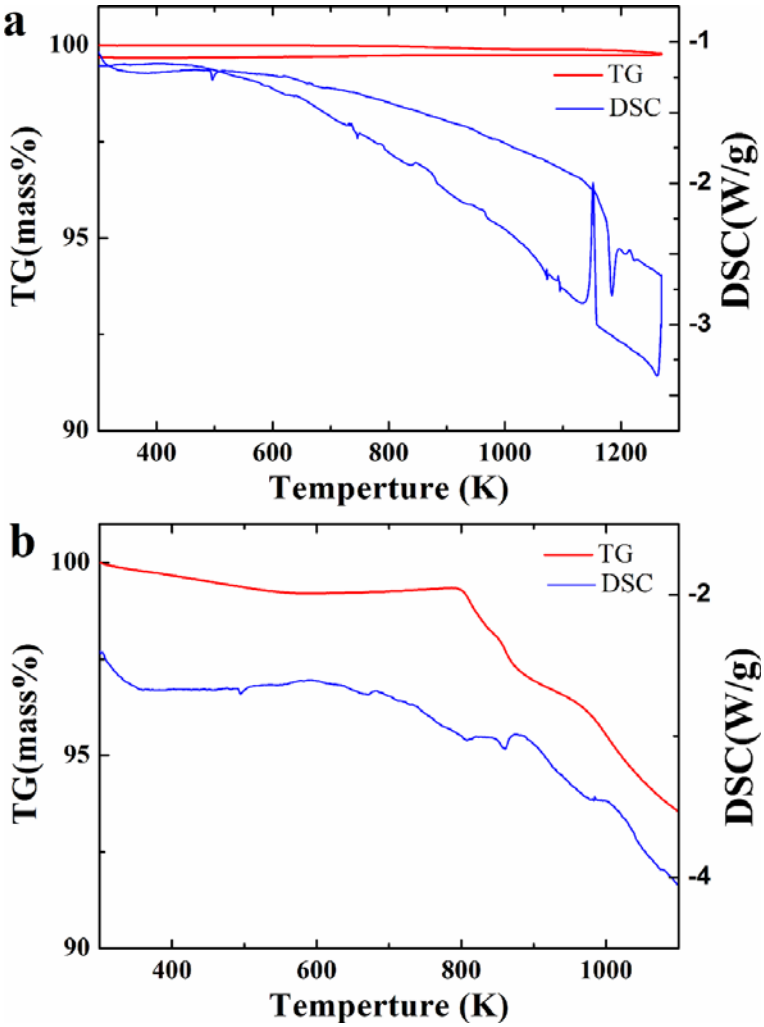

Figure S1. TG-DSC measurements on (a) α-$Sr_3Sn_2As_4$ and (b) β-$Sr_3Sn_2As_4$, conducted in an inert atmosphere of argon.

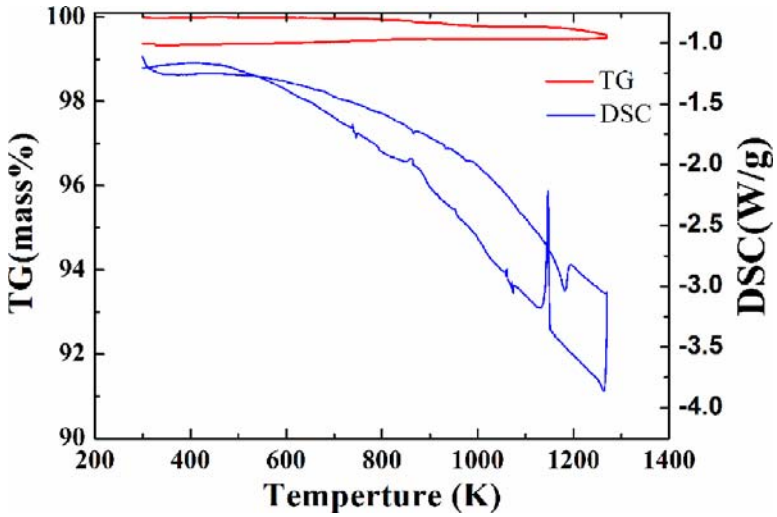

Figure S2. The 2nd cycle of TG-DSC curves for α-$Sr_3Sn_2As_4$.

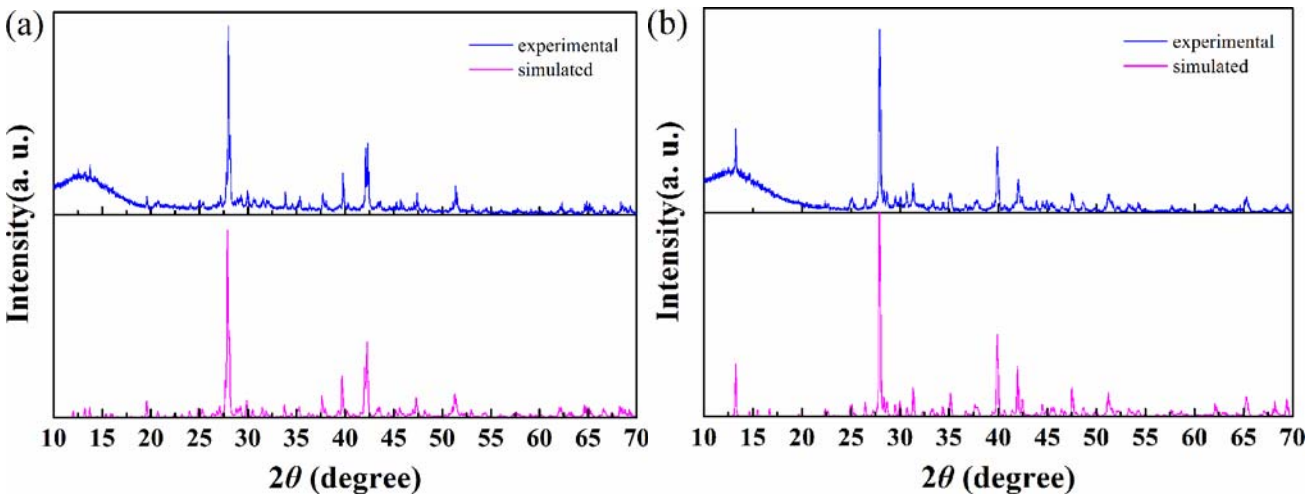

Figure S3. Experimental (blue) and simulated (red) X-ray powderdi□raction data of (a) α and (b) β-$Sr_3Sn_2As_4$.

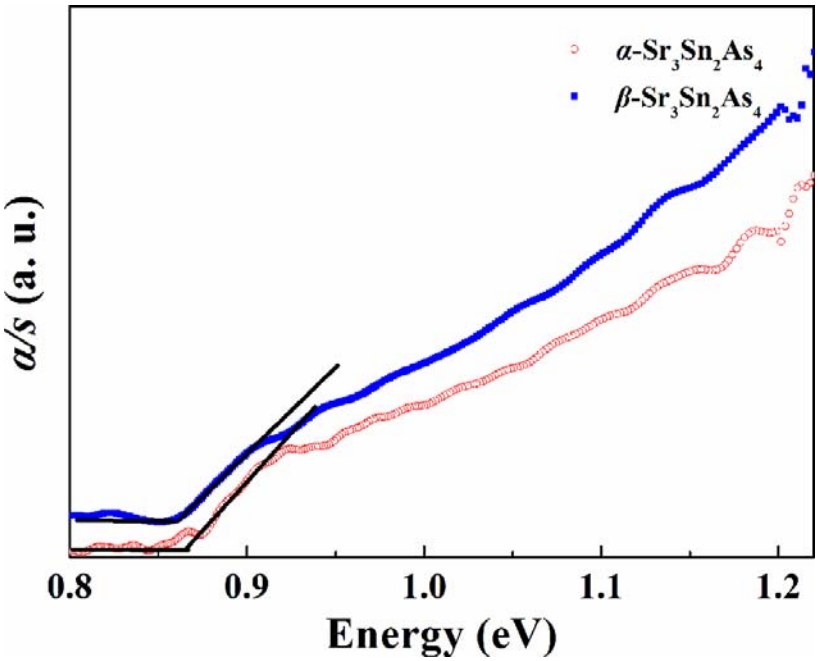

Fig. S4. Optical absorption spectrum measured on polycrystalline samples of α-$Sr_3Sn_2As_4$ and β-$Sr_3Sn_2As_4$.

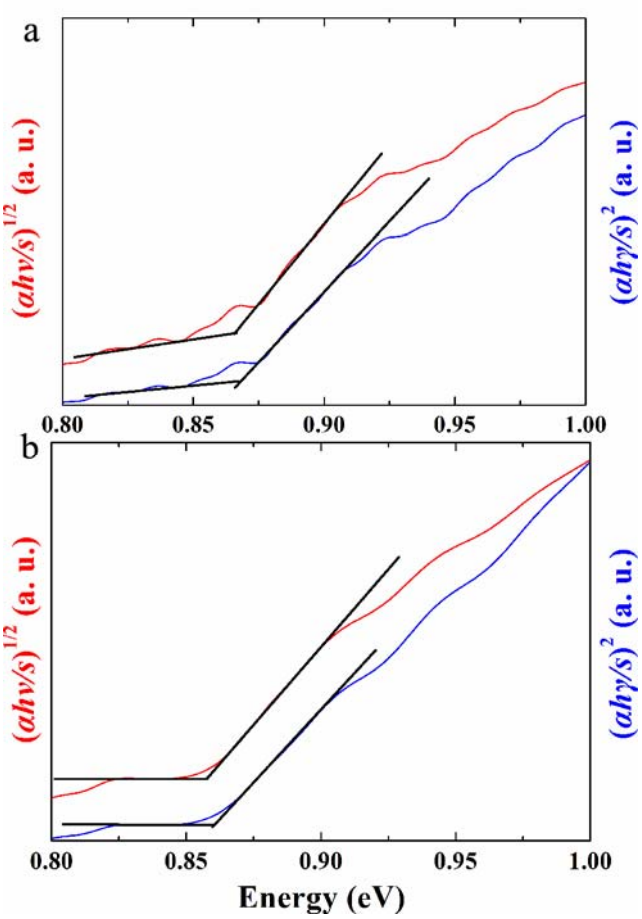

Fig. S5. Tauc plots for (a) α and (b) β-$Sr_3Sn_2As_4$ at room temperature. The linear fits of $(\alpha hv/S)^{1/2}$ and $(\alpha hv/S)^2$ vs hv plots are used for the calculation of indirect and direct band gaps, respectively.

Table S1. Refined atomic coordinates and isotropic displacement parameters for two polymorphs of $Sr_3Sn_2As_4$.

Atoms	*Wyckoff site*	*x*	*y*	*z*	*Ueq (Å^2)*
α-$Sr_3Sn_2As_4$					
Sr1	*16g*	0.08386(3)	0.28712(7)	0.13070(4)	0.01087(18)
Sr2	*16g*	0.16857(3)	0.04676(7)	0.25739(4)	0.01059(18)
Sr3	*16g*	0.25560(3)	0.28834(7)	0.12717(4)	0.01242(19)
Sr4	*8f*	0	0.05958(10)	0.27092(6)	0.0117(3)
Sr5	*8d*	0.32523(4)	0	0	0.0107(3)
Sr6	*4b*	1/2	0	0	0.0089(3)
Sr7	*4a*	0	0	0	0.0151(4)
Sn1	*16g*	0.08543(2)	0.34615(5)	0.32211(3)	0.00896(14)
Sn2	*16g*	0.16206(2)	0.06286(5)	0.05956(3)	0.00878(14)
Sn3	*16g*	0.41779(2)	0.20947(5)	0.06648(3)	0.00883(14)
As1	*16g*	0.07605(3)	0.03920(8)	0.13393(4)	0.0107(2)
As2	*16g*	0.08743(4)	0.02573(7)	0.38306(4)	0.01018(19)
As3	*16g*	0.16529(4)	0.29709(8)	0.24765(5)	0.01046(19)
As4	*16g*	0.16645(4)	0.25313(7)	0.00822(5)	0.0102(2)
As5	*16g*	0.24690(3)	0.03843(8)	0.12620(4)	0.0102(2)
As6	*8f*	0	0.24804(10)	0.01211(6)	0.0093(3)

As7	*8f*	0	0.30939(11)	0.24880(6)	0.0102(3)
β-$Sr_3Sn_2As_4$					
Sr1	*4e*	0.21062(11)	0.81719(4)	0.00999(11)	0.01116(17)
Sr2	*4e*	0.25910(10)	0.56067(4)	0.01154(10)	0.01029(17)
Sr3	*4e*	0.26307(11)	0.06093(4)	0.00586(10)	0.01097(17)
Sn1	*4e*	0.20769(8)	0.37681(3)	0.02819(8)	0.01473(15)
Sn2	*4e*	0.32032(7)	0.24274(3)	0.41053(7)	0.00972(14)
As1	*4e*	0.00169(12)	0.55548(4)	0.25618(11)	0.01207(18)
As2	*4e*	0.02632(12)	0.31749(4)	0.21937(12)	0.01115(18)
As3	*4e*	0.50580(11)	0.43522(4)	0.25118(11)	0.01124(18)
As4	*4e*	0.52427(12)	0.19502(4)	0.22712(11)	0.00969(17)

[a] U_{eq} is defined as one third of the trace of the orthogonalized U^{ij} tensor

Table S2. Important interatomic distances (Å) in two polymorphs of $Sr_3Sn_2As_4$

Atom pairs	Distances (Å)	Atom pairs	Distances (Å)
α-$Sr_3Sn_2As_4$			
Sr1 – As1	3.2022(14)	Sr2 – As1	3.3586(12)
As2	3.0879(13)	As2	3.1985(12)
As3	3.0713(12)	As3	3.2204(14)
As4	3.1968(12)	As3	3.2328(14)
As6	3.1745(12)	As5	3.1183(12)
As7	3.1407(12)	As5	3.2234(12)
Sr3 – As3	3.1479(12)	Sr4 – As1×2	3.2835(13)
As3	3.2786(13)	As2×2	3.1427(12)
As4	3.2665(12)	As7	3.2466(19)
As4	3.3217(13)	As7	3.2472(19)
As5×2	3.2289(14)	Sr6 – As2×4	3.1936(9)
Sr5 – As2×2	3.1920(12)	As6×2	3.2556(14)
As4×2	3.1928(10)	Sr7 – As1×4	3.2659(9)
As5×2	3.1865(11)	As6×2	3.2052(14)
Sn1 – Sn3	2.7659(9)	Sn2 – Sn2	2.7955(12)
As1	2.6374(12)	As1	2.6531(10)
As3	2.5830(11)	As4	2.6440(12)
As7	2.6547(9)	As5	2.5523(10)
Sn3 – As2	2.5608(11)		
As4	2.6451(11)		

	As6	2.6563(9)			
β-$Sr_3Sn_2As_4$					
Sr1 –	As1	3.1577(12)	Sr2 –	As1	3.1790(12)
	As2	3.2416(12)		As1	3.2055(12)
	As2	3.2649(12)		As2	3.2385(12)
	As3	3.1987(12)		As3	3.1793(11)
	As4	3.2155(11)		As3	3.1836(12)
	As4	3.2585(12)		As4	3.3026(11)
Sr3 –	As1	3.1300(12)	Sn1 –	Sn2	2.7173(9)
	As1	3.2118(12)		As1	2.5327(11)
	As2	3.2512(12)		As2	2.6340(11)
	As3	3.1533(12)		As3	2.5517(10)
	As3	3.1748(11)	Sn2 –	As2	2.6151(10)
	As4	3.3091(12)		As4	2.6350(10)
				As4	2.6362(10)