Supporting Information

Synthesis and Thermoelectric Properties of Copper Sulfides via Solution Phase Methods and Spark Plasma Sintering

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1. XRD refinement

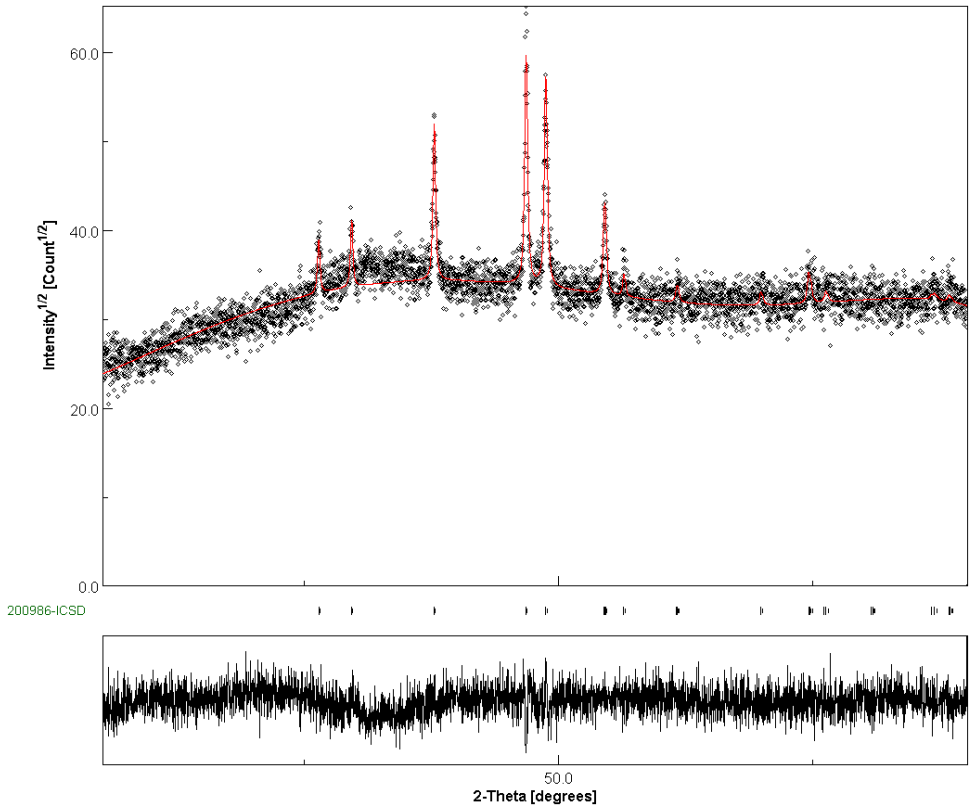

Figure S1 XRD refinement patterns of the hexagonal Cu_2S powder sample

The powder XRD refinement for the hexagonal Cu_2S sample as shown in Fig .S1. The lower error values (Sig=1.487875 and Rwp (%) =5.4611034) were obtained, indicating that the refinement result is reliable. In the refinement process, we choose the model ICSD#200986, which correspond to the standard card (JSPDS no. 26-1116). The location, proportion and lattice constant of experiment and

refinement Cu ions as shown in table S1. In the refinement process, we fixed the position of sulfur ions, and let the location and proportion of Cu ions can be refine. Obvious, the proportion of Cu 1 changed from 0.75 to 0.4896, indicted that there are more Cu vacancies, the smaller lattice parameters and possibility of defects in hexagonal Cu_2S.

Table S1 The location, proportion and lattice constant of Cu ions

	experiment			refinement		
	location	proportion	lattice constant	location	proportion	lattice constant
Cu 1	0 0 0.25	0.75	a=3.959	-2.89E-4 -1.10E-5 0.2495	0.4896	a=3.882
Cu 2	0.2573 0.5146 0.4339	0.2158	c=6.764	0.2578 0.5146 0.4427	0.2038	c=6.745

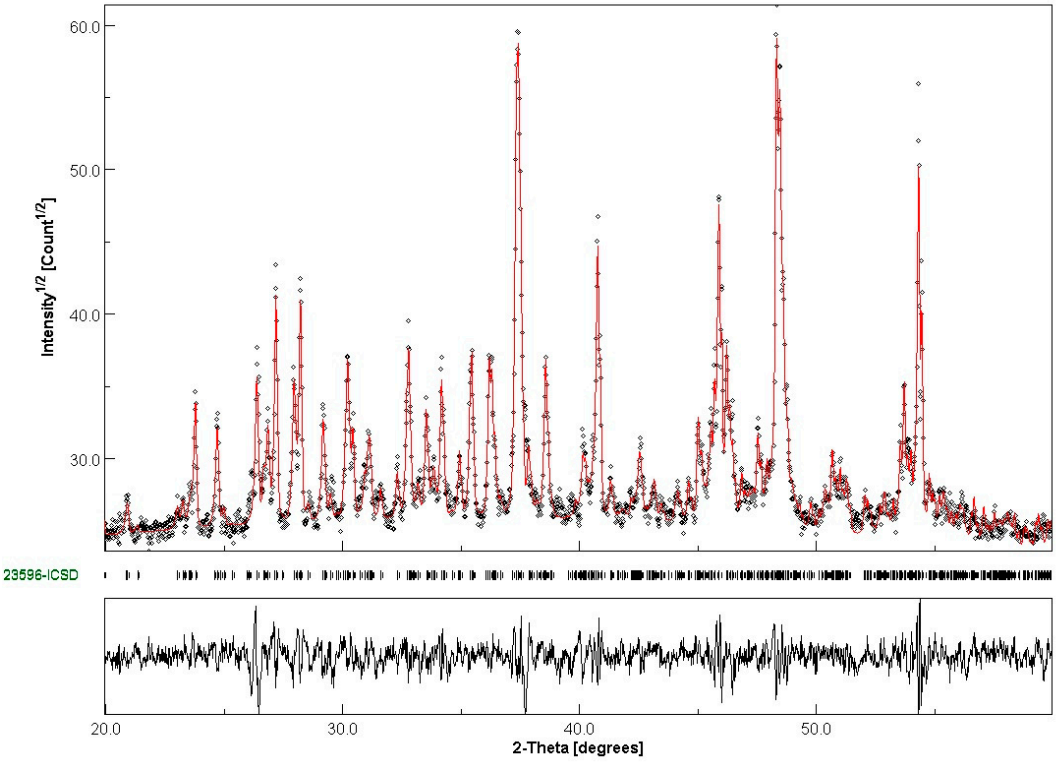

Figure S2 XRD refinement patterns of the monoclinic Cu_2S powder sample

Table S2 The lattice constant of monoclinic Cu_2S powder sample

lattice constant	experiment	refinement
a	15.246	15.247603
b	11.884	11.896455
c	13.494	13.498567
angle	116.35	116.29502

We did powder XRD refinement for the monoclinic Cu_2S sample as shown in Fig .S2. The lower error values (Sig=1.487875 and Rwp (%) =5.4611034) were obtained, indicating that the refinement result is reliable. In the refinement process, we choose the model ICSD#23596, which correspond to the standard card (JSPDS no. 83-1462), and we opened the option of texture.

The lattice constant of monoclinic Cu_2S sample as shown in table S2. There is no obvious different between refinement and experiment values. Indicated that the diffraction peaks are well matched. The monoclinic samples have impurity no peaks but have some textures.