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Supporting information for article:

Structural evolution of a Ge-substituted SnSe thermoelectric material with low thermal conductivity

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Table S1. Crystallographic data for $Sn_{0.9}Ge_{0.2}Se$ from NPD data at 473 K.

Crystal data

Orthorhombic	**Space group: *Pnma***
Hall symbol: -P 2ac 2n	Constant wavelength neutron diffraction radiation, λ = 1.594 Å
a = 11.5376 (12) Å	T = 473 K
b = 4.1694 (4) Å	Particle morphology: powder
c = 4.4254 (4) Å	
V = 212.88 (3) Å^3	
Z = 4	Specimen preparation: arc melting from Sn+Se+Ge

Refinement: Rietveld	**68 parameters**
R_p = 2.41%5	
R_{wp} = 3.22%	
R_{exp} = 1.72%	
R_{Bragg} = 4.09%	
χ^2 = 3.63%	
3198 data points	Background function: Linear interpolation between a set of background points with refinable heights
Excluded region(s): 0	Preferred orientation correction: Yes
Profile function:	Pseudo Voigt

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	***y***	***z***	U_{iso}*/U_{eq}	**Occ. (<1)**
Sn1	0.11859 (18)	0.25000	0.0977 (4)	0.0324 (15)	
Ge1	0.11859 (18)	0.25000	0.0977 (4)	0.0324 (15)	0.20000
Se1	0.35498 (15)	0.25000	0.0197 (3)	0.0228 (8)	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.0358 (18)	0.0280 (14)	0.0335 (12)	0.00000	−0.0049 (9)	0.00000

Ge1	0.0358 (18)	0.0280 (14)	0.0335 (12)	0.00000	−0.0049 (9)	0.00000
Se1	0.0243 (10)	0.0203 (7)	0.0239 (7)	0.00000	−0.0022 (7)	0.00000

Table S2. Crystallographic data for $Sn_{0.9}Ge_{0.2}Se$ from NPD data at 693 K.

Crystal data

Orthorhombic	**Space group: *Pnma***
Hall symbol: -P 2ac 2n	Constant wavelength neutron diffraction radiation, λ = 1.594 Å
a = 11.6239 (18) Å	T = 693 K
b = 4.2297 (6) Å	Particle morphology: powder
c = 4.3742 (7) Å	
V = 215.06 (6) Å^3	
Z = 4	Specimen preparation: arc melting from Sn+Se+Ge

Refinement: Rietveld	**70 parameters**
R_p = 2.29%	
R_{wp} = 3.07%	
R_{exp} = 1.73%	
R_{Bragg} = 4.42%	
χ^2 = 3.26	
3198 data points	Background function: Linear interpolation betv a set of background points with refinable heigh
Excluded region(s): 0	Preferred orientation correction: Yes
Profile function:	Pseudo Voigt

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	***y***	***z***	***U*$_{iso}$*/*U*$_{eq}$**	**Occ. (<1)**
Sn1	0.1219 (2)	0.25000	0.0800 (5)	0.048 (2)	
Ge1	0.1219 (2)	0.25000	0.0800 (5)	0.048 (2)	0.20000

Se1	0.3567 (2)	0.25000	0.0142 (4)	0.0348 (11)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.060 (3)	0.0436 (19)	0.0386 (15)	0.00000	−0.0016 (15)	0.00000
Ge1	0.060 (3)	0.0436 (19)	0.0386 (15)	0.00000	−0.0016 (15)	0.00000
Se1	0.0371 (13)	0.0297 (10)	0.0375 (11)	0.00000	−0.0008 (12)	0.00000

Table S3. Crystallographic data for $Sn_{0.9}Ge_{0.2}Se$ from NPD data at 853 K.

Crystal data

Orthorhombic	**Space group: *Cmcm***
Hall symbol: -C 2c 2	Constant wavelength neutron diffraction radiation, λ = 1.594000 Å
a = 4.2999 (6) Å	T = 853 K
b = 11.7110 (18) Å	Particle morphology: powder
c = 4.3097 (6) Å	
V = 217.02 (6) Å^3	
Z = 4	Specimen preparation: arc melting from Sn+Se+Ge

Refinement: Rietveld	**79 parameters**
R_p = 2.965	
R_{wp} = 4.234	
R_{exp} = 1.744	
R_{Bragg} = 6.421	
χ^2 = 6.178	
3197 data points	Background function: Linear interpolation between a set of background points with refinable heights

Excluded region(s): 0	Preferred orientation correction: Yes
Profile function:	Pseudo Voigt

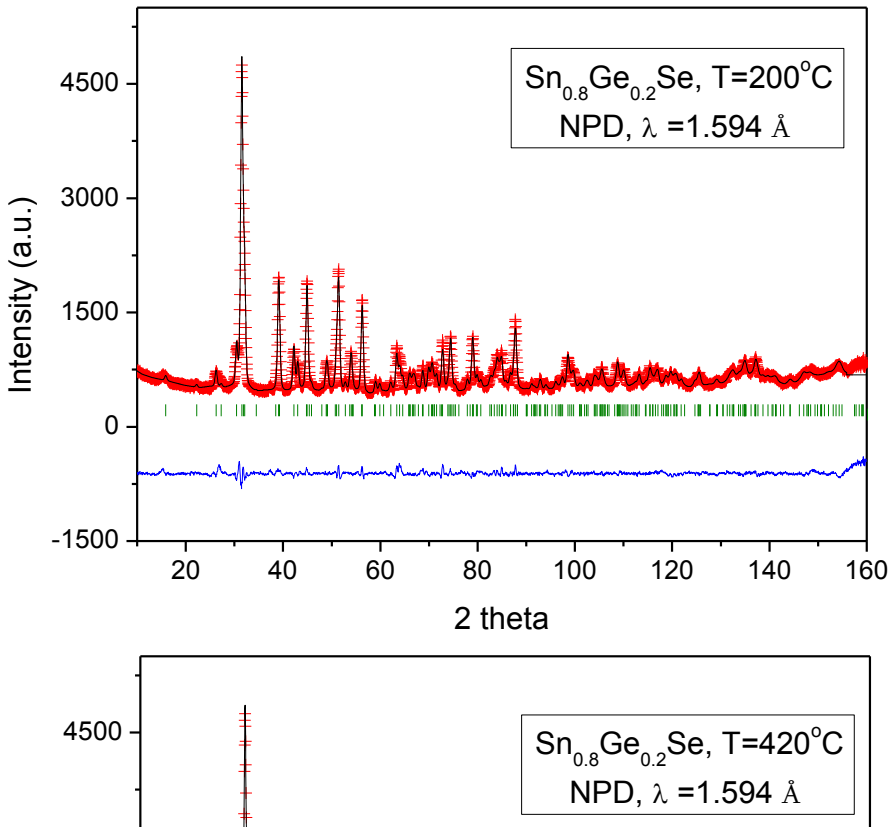
Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

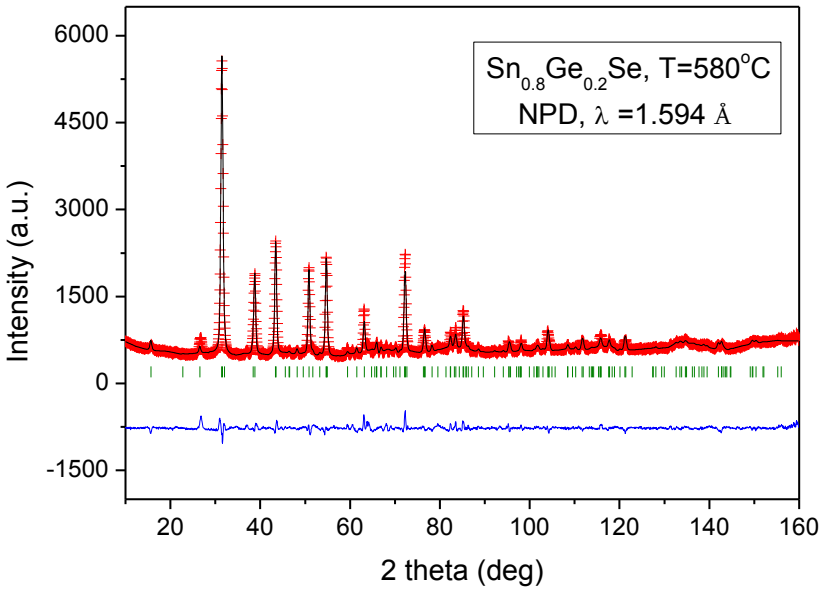
	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Sn1	0.00000	0.3747 (4)	0.25000	0.088 (4)	
Ge1	0.00000	0.3747 (4)	0.25000	0.088 (4)	0.20000
Se1	0.00000	0.1399 (3)	0.25000	0.0439 (18)	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.057 (4)	0.152 (5)	0.056 (3)	0.00000	0.00000	0.00000
Ge1	0.057 (4)	0.152 (5)	0.056 (3)	0.00000	0.00000	0.00000
Se1	0.0124 (17)	0.0712 (19)	0.048 (2)	0.00000	0.00000	0.00000

Fig. S1. Rietveld plots for $Sn_{0.9}Ge_{0.2}Se$ at (a) 473 K, (b) 693 K and (c) 853 K.




Sn0.8Ge0.2Se, T=580°C
NPD, λ =1.594 Å
Intensity (a.u.)
2 theta (deg)
6000
4500
3000
1500
0
-1500
20
40
60
80
100
120
140
160