Ba-filled Ni-Sb-Sn based Skutterudites with anomalously high lattice thermal conductivity

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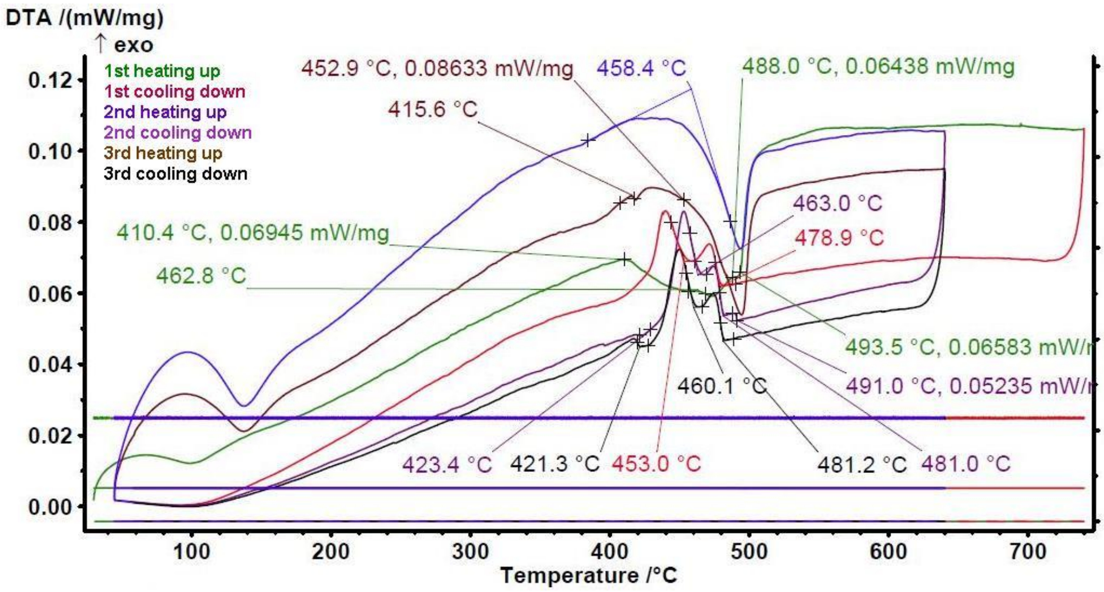

Figure I: DTA curves of the single phase-sample $Ni_4Sb_{8.2}Sn_{3.8}$.

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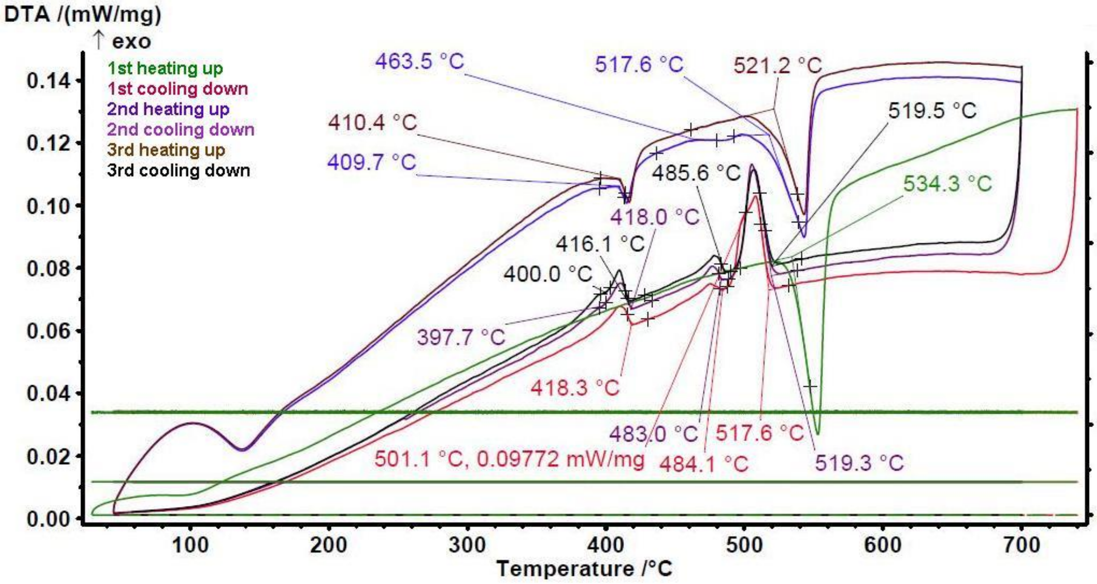

Figure II: DTA curves of the single-phase sample $Ba_{0.29}Ni_4Sb_{9.1}Sn_{2.9}$.

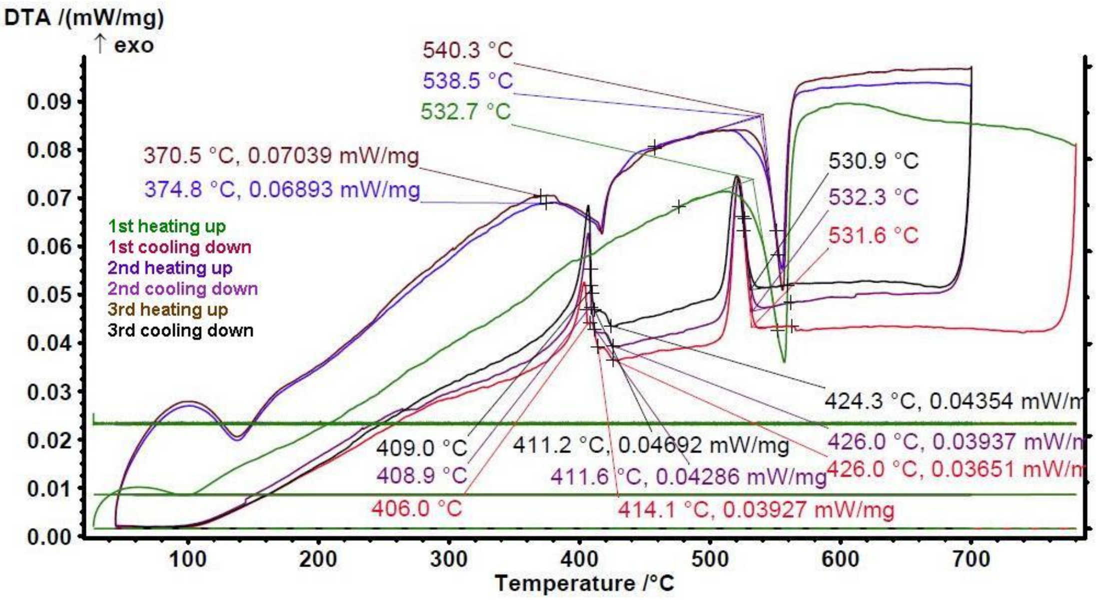

Figure 3.III: DTA curves of the single-phase sample $Ba_{0.42}Ni_4Sb_{8.2}Sn_{3.8}$.

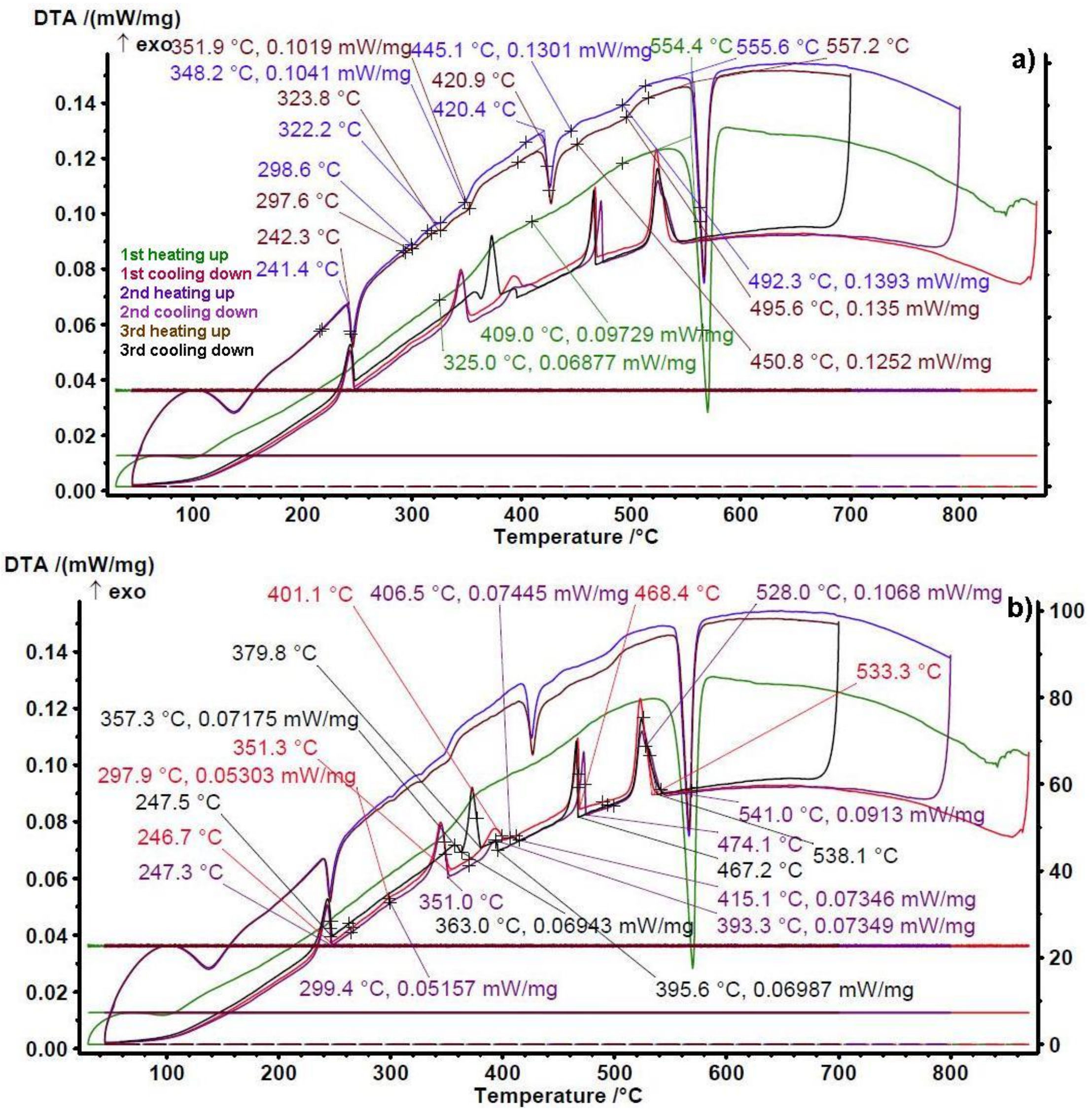

Figure 3IV: DTA curves of the single-phase sample $Ba_{0.92}Ni_4Sb_{6.7}Sn_{5.3}$. Curves are shown twice a) and b) to present all the evaluated temperatures for the occurring thermal effects.

Table I: Temperature dependent ^{119}Sn Mössbauer parameters, i.e. isomer shift δ, quadrupole splitting ΔE_Q and linewidth Γ. Component I, II, and III represent the different possible coordinations of Sn with 2, 1, or 0 Sb next neighbors.

sample	temperature	component	δ (mm/s)	ΔE_Q (mm/s)	Γ (mm/s)
$Ni_4Sb_{8.2}Sn_{3.8}$	290	I	2.47(6)	0.94(6)	0.88(5)
		II	2.71(7)	0.82(9)	1.0(1)
	200	I	2.44(1)	0.95(1)	0.84(2)
		II	2.65(2)	0.85(2)	0.88(3)
	100	I	2.45(1)	0.94(1)	0.83(1)
		II	2.71(1)	0.89(1)	0.91(2)
	10	I	2.43(1)	0.93(1)	0.85(1)
		II	2.75(1)	0.91(1)	0.91(1)
$Ba_{0.29}Ni_4Sb_{9.2}Sn_{2.9}$	290	I	2.53(1)	1.07(2)	0.77(1)
		II	2.56(1)	0.55(2)	0.75(5)
	200	I	2.56(1)	1.13(1)	0.77(1)
		II	2.57(1)	0.53(1)	0.68(2)
	75	I	2.59(1)	1.14(2)	0.78(2)
		II	2.57(1)	0.54(1)	0.66(3)
	10	I	2.58(1)	1.15(1)	0.81(1)
		II	2.58(1)	0.85(1)	0.68(2)
$Ba_{0.42}Ni_4Sb_{8.2}Sn_{3.8}$	290	I	2.41(1)	0.91(1)	0.77(1)
		II	2.64(1)	0.89(1)	0.82(2)
	200	I	2.42(1)	0.91(1)	0.82(2)
		II	2.70(1)	0.90(1)	0.80(1)
	100	I	2.45(1)	0.89(1)	0.82(2)
		II	2.71(1)	0.90(1)	0.82(2)
	10	I	2.44(1)	0.91(1)	0.80(1)
		II	2.73(1)	0.90(1)	0.81(2)
$Ba_{0.92}Ni_4Sb_{6.7}Sn_{5.3}$	290	I	2.30(9)	0.8(1)	0.9(1)
		II	2.53(3)	0.98(3)	0.82(3)
		III	2.56(9)	0.5(1)	0.8(1)
	200	I	2.44(5)	0.9(1)	1.0(1)
		II	2.55(2)	1.00(3)	0.83(3)
		III	2.56(4)	0.46(5)	0.70(7)
	100	I	2.42(4)	0.83(5)	0.96(7)
		II	2.58(2)	1.02(3)	0.85(2)
		III	2.60(3)	0.48(5)	0.71(5)
	10	I	2.41(6)	0.85(8)	0.97(8)
		II	2.55(3)	1.02(3)	0.85(2)
		III	2.61(5)	0.44(7)	0.75(8)

Table II: ^{121}Sb Mössbauer parameters at 10 K, i.e. isomer shift δ, quadrupole splitting ΔE_Q and linewidth Γ.

sample	**δ (mm/s)**	**ΔE_Q (mm/s)**	**Γ (mm/s)**
$Ni_4Sb_{8.2}Sn_{3.8}$	-1.2(1)	3.1(5)	2.9(2)
$Ba_{0.29}Ni_4Sb_{9.2}Sn_{2.9}$	-1.3(1)	2.7(7)	3.2(2)
$Ba_{0.42}Ni_4Sb_{8.2}Sn_{3.8}$	-1.2(1)	2.6(8)	3.1(2)
$Ba_{0.92}Ni_4Sb_{6.7}Sn_{5.3}$	-1.0(1)	3.1(5)	3.0(1)