SUPPORTING INFORMATION (SI)

Enhanced power factor and suppressed lattice thermal conductivity of $CoSb_3$ Skutterudite by Ni substitution and nanostructuring for high thermoelectric performance

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Table S1: Cp values of pure and Ni substituted samples as a function of temperature.

Temperature (K)	**Cp (J/g*K) for Pure**	**Cp (J/g*K) for $Co_{0.98}Ni_{0.02}Sb_3$**	**Cp (J/g*K) for $Co_{0.96}Ni_{0.04}Sb_3$**	**Cp (J/g*K) for $Co_{0.94}Ni_{0.06}Sb_3$**
323	0.659	0.546	0.430	0.316
384	0.694	0.583	0.476	0.372
423	0.696	0.612	0.529	0.446
483	0.733	0.649	0.568	0.487
523	0.711	0.656	0.605	0.551
544	0.756	0.702	0.649	0.597

Table S2. Represent the crystallite size (nm), microstrain (ε) and dislocation density (δ) of the prepared material.

Sample	**Crystallite size (nm)**	**Microstrain(ε)**	**Dislocation density (δ) (lines/nm²)**
Pure $CoSb_3$	48.52	0.151	4.2×10^{-4}
$Co_{0.98}Ni_{0.02}Sb_3$	48.52	0.151	4.2×10^{-4}
$Co_{0.96}Ni_{0.04}Sb_3$	43.41	0.169	5.3×10^{-4}

$Co_{0.94}Ni_{0.06}Sb_3$	45.83	0.159	4.7×10^{-4}
$Co_{0.92}Ni_{0.08}Sb_3$	44.34	0.165	5.0×10^{-4}

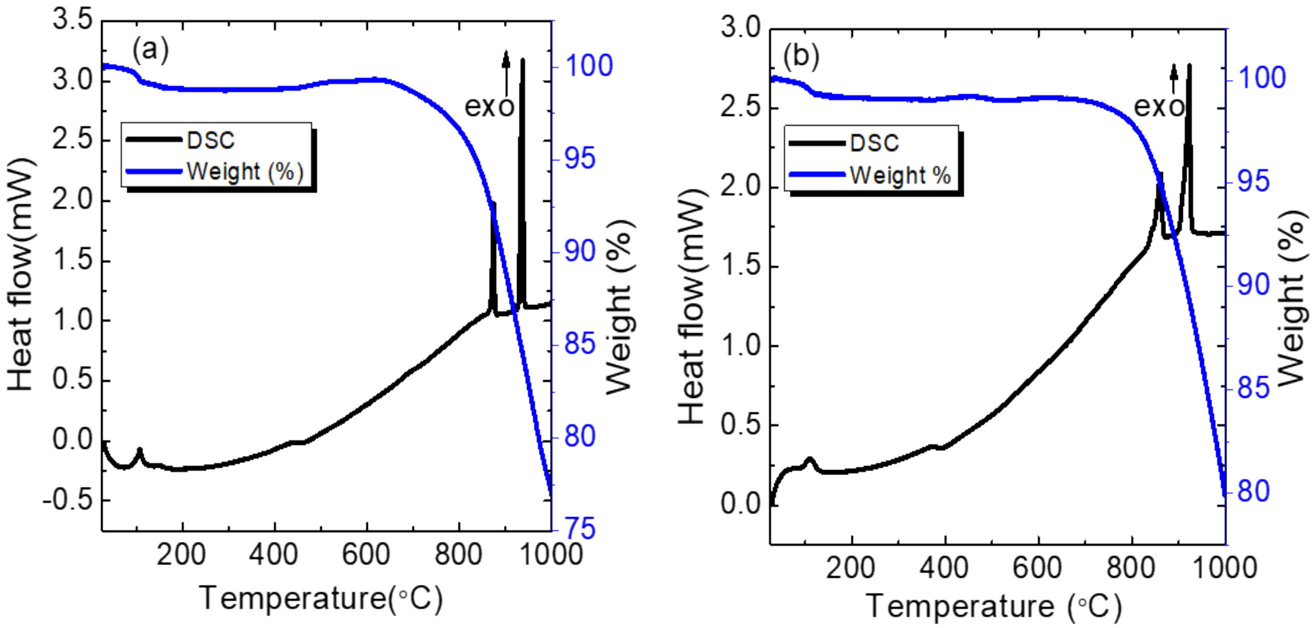

Figure S1 TGA /DSC of (a) pure $CoSb_3$ and (b) $Co_{0.94}Ni_{0.06}Sb_3$ samples.

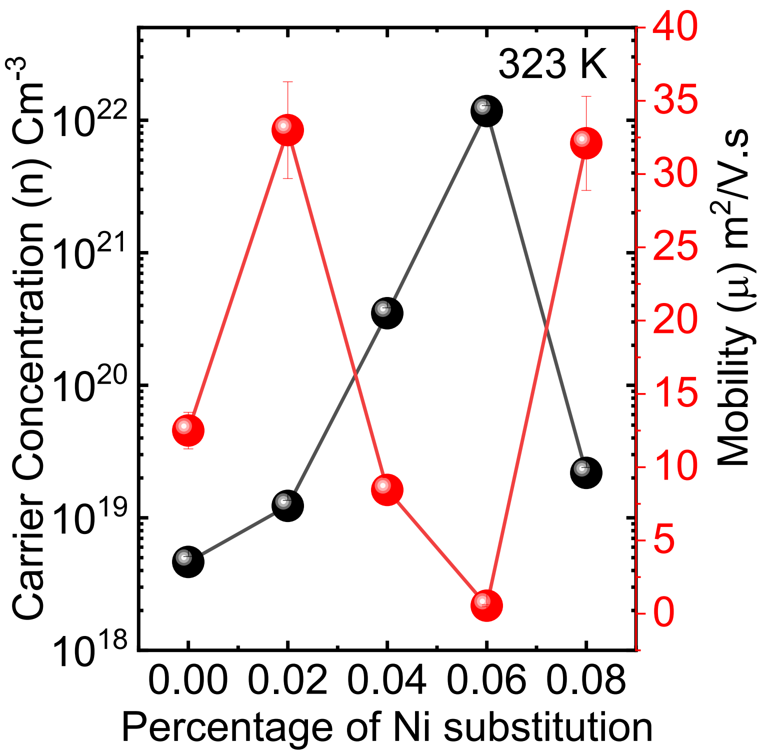

Figure S2 Variation of Carrier concentration (n) and mobility (μ) of the Ni substituted samples as a function of Ni content at 323 K.

Table S3. Comparison of Thermoelectric parameters with the previous literatures of similar materials.

Materials	**σ (Ωm)$^{-1}$**	**S (μV/K)**	**Power Factor (W/mK^2)**	**κ (W/mK)**	**zT**	**References**
$Co_{0.93}Ni_{0.07}Sb_3$	10^5	-194	-	0.5	0.2 at 650 K	[31]
$Bi_{0.5}Co_4Sb_{12}$	3×10^4	-205	$1.4{\times}10^{-3}$	3.02	0.53 at 632K	[51]
$CoSb_3$	$19{\times}10^4$	155	$1.4{\times}10^{-3}$	1.6	0.47 at 660K	[52]

$Co_{0.95}Ni_{0.05}Sn_{1.5}Te_{1.5}$	2	-250	1.9×10^{-3}	2	0.73 at 773K	[53]
$Se_{0.05}Ni_{0.4}Co_{3.6}Sb_{12}$	8×10^{4}	-103	2.7×10^{-3}	3.4	0.71 at 823K	[54]
$Co_{0.91}Ni_{0.09}Sb_{3}$	7×10^{4}	-150	-	3.2	0.70 at 573K	[55]
$S_{0.25}Co_{3.4}Ni_{0.6}Sb_{12}$	17.9×10^{4}	-170	3.4×10^{-3}	2.7	0.81 at 800K	[30]
$Dy_{0.4}Co_{3.2}Ni_{0.8}Sb_{12}$	1.63×10^{5}	-180	5.2×10^{-3}	2.3	1.4 at 773K	[25]
$Ba_{0.08}La_{0.05}Yb_{0.04}Co_{4}Sb_{12}$	2.39×10^{4}	-126	5.5×10^{-3}	2.7	1.7 at 850K	[24]
$0.2Co/Ba_{0.3}In_{0.3}Co_{4}Sb_{12}$	13×10^{4}	-210	-	2.6	1.8 at 850K	[23]
$Co_{0.94}Ni_{0.06}Sb_{3}$	1.16×10^{5}	-213	5.27×10^{-3}	3.6	0.78 at 553K	Present work
$Co_{0.96}Ni_{0.04}Sb_{3}$	5.44×10^{4}	-342	6.40×10^{-3}	2.0	1.72 at 553K	Present work