

## Enhancement of Thermoelectric Properties of Yb-filled Skutterudites by Ni Induced “Core-shell” Structure

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### XRD patterns

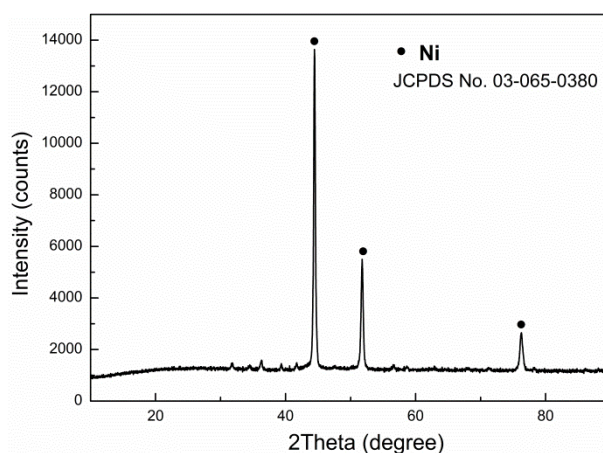


Figure S1 the XRD pattern of the product of thermal decomposition of nickel acetate under the special reducing gas.

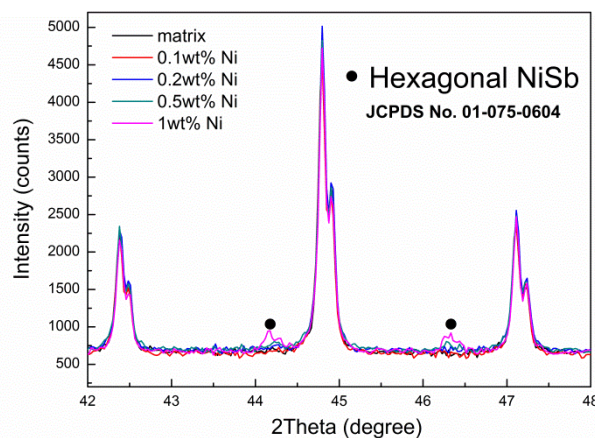


Figure S2 the XRD pattern of the studied samples in the 2Theta range of 42 to 48 degrees. The pattern of 1wt% Ni sample is also shown.

Table S1: the normalized compositions of the randomly selected normal and nano grains in matrix sample and 0.2wt% Ni sample.

	Grain number	Yb	Co	Ni	Sb
Normal grain 1	1	0.15	3.69	--	12
Normal grain 2	2	0.11	3.97	--	12
Normal grain 3	3	0.13	3.89	--	12
Normal grain 4	4	0.08	3.62	--	12
Nano grain 1	5	0.10	3.78	0.06	12
Nano grain 2	6	0.14	3.57	0.10	12
Nano grain 3	7	0.18	3.52	0.11	12

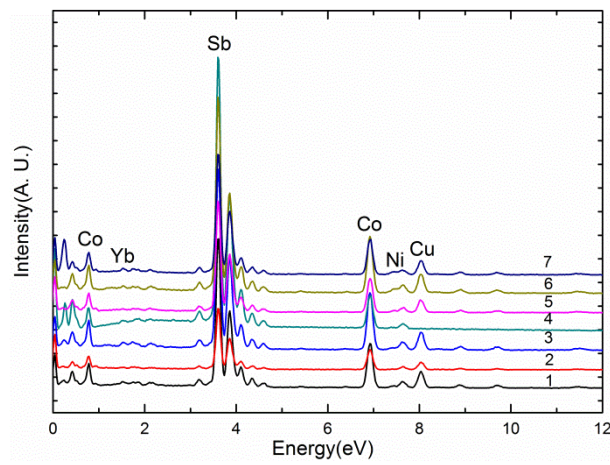


Figure S3 The EDS curves corresponding to the grains in Table S1. The appearance of Cu peak in the profiles is due to the copper ring used for sample supporting for the TEM analysis. The line of 4 is obtained on the matrix sample in the SEM equipped with an EDS detector on which the Cu peak is absent.

Table S2 Input parameters for calculation of relaxation time rate of phonon scattering for 0.2wt% Ni sample.

Relaxation time rate	Parameter	Symbol	Value
$\tau_U^{-1} \approx \frac{\hbar\gamma^2}{Mv^2\theta_D} \omega^2 T \exp(-\theta_D/3T)$ [4]	Gruneisen parameter of 0.2wt% Ni sample	$\gamma$	0.95 [1]
	Average sound velocity of 0.2wt% Ni sample	v(m/s)	2934 [1]
	Debye temperature of 0.2wt% Ni sample	$\theta_D$ (K)	311 [2]
	Average mass of an atom of 0.2wt% Ni sample	M (kg)	$1.776 \times 10^{-25}$
$\tau_N^{-1} \approx \beta \tau_U^{-1}$	Ration of normal phonon scattering to Umklapp scattering	$\beta$	2.75 [3]
$\tau_{PD}^{-1} \approx x(1-x) \frac{M(Yb)}{M}$ [3] $M = 4M(Co) + 12M(Sb) + 0.2M(Yb)$ Neglecting the mass fluctuation from Ni substitution for Co	Mass of an atom Co	M(Co) (g/mol)	58.9332
	Mass of an atom Sb	M(Sb) (g/mol)	121.76
	Mass of an atom Yb	M(Yb) (g/mol)	173.04
	Mass of 0.2wt% Ni sample	M (g/mol)	1731.4608
$\tau_B^{-1} = \frac{v}{L}$ [5]	The grain size	L (nm)	120 for the nanograins; 6000 for the normal grains
$\tau_R^{-1} = \frac{C\omega^2}{(\omega_0^2 - \omega^2)^2}$ [5]		C (s <sup>-3</sup> )	$3.072 \times 10^{33}$ [5]
	Resonance frequency	$\omega_0$ (THz)	3.409 [5]

## References

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