Reduced thermal conductivity and electrical resistivity in Bi_2Se_3 thermoelectric compounds: Effect of In and Te Co-doping

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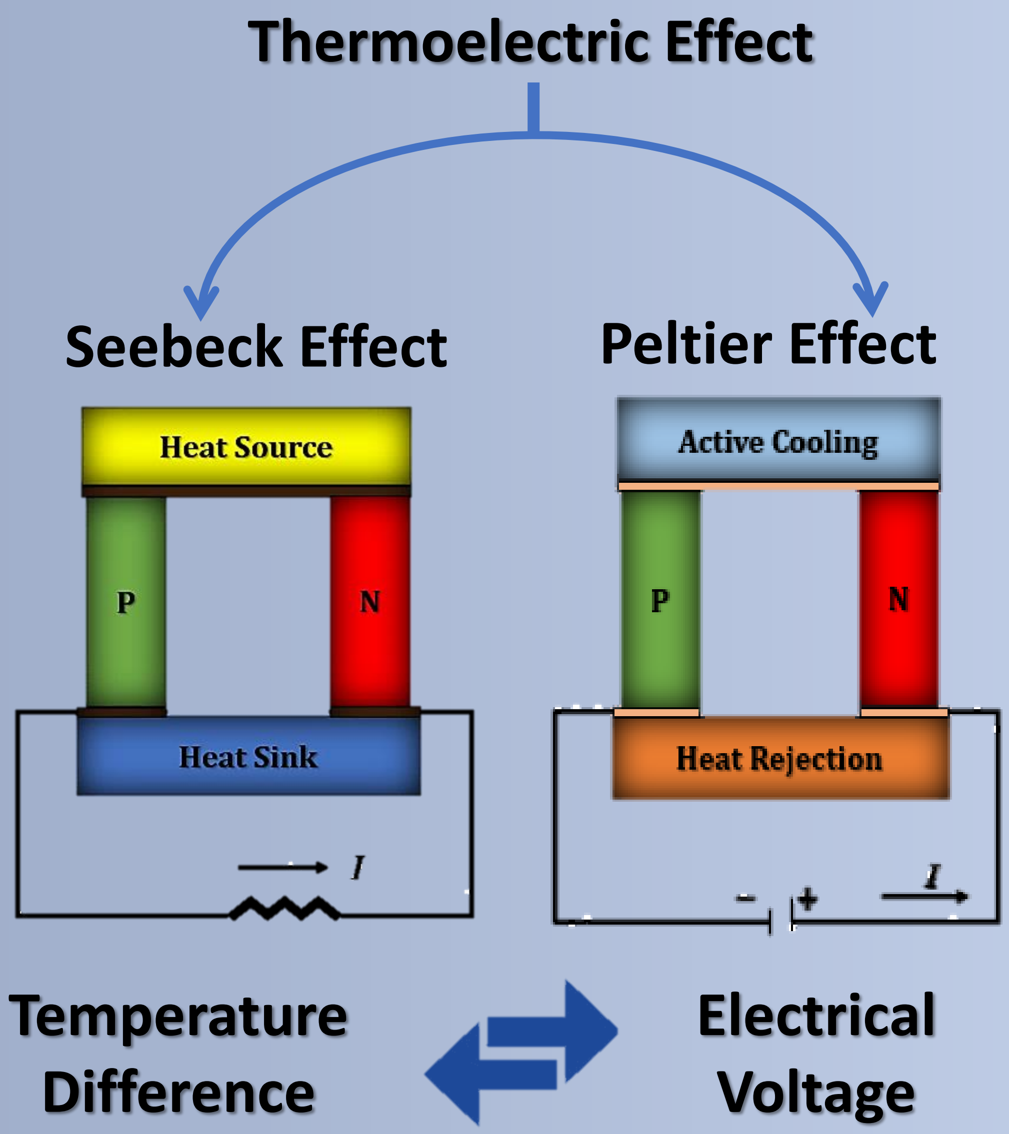


Methodology

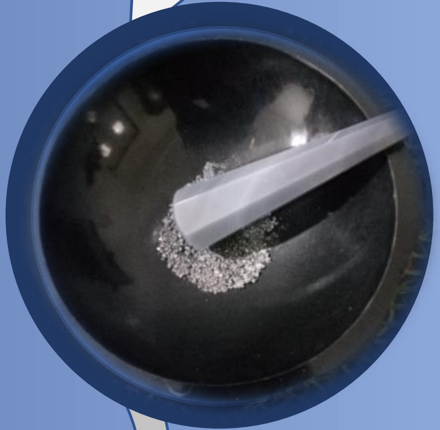
1. Grinding for 2 Hours

2. Pelletizing under 5 Ton Compression

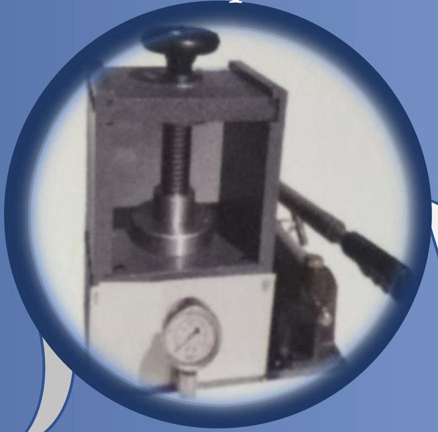
3. Vacuum Sealing at 10^{-6} Torr

4. Sintering at 420^{0}C for 24 Hours

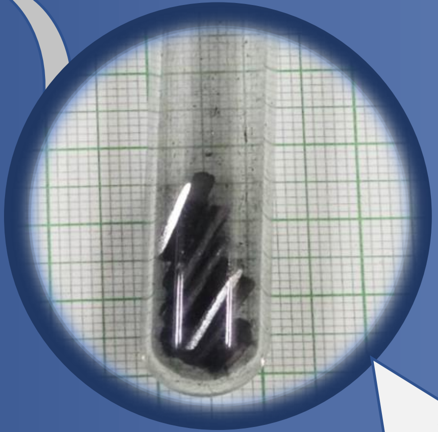
5. Regrinding for 1 Hour



6. Pelletizing under 5 Ton Compression



7. Vacuum Sealing at 10^{-6} Torr



8. Sintering at 200^{0}C for 12 Hours

Samples

Characterizations

Powder X-ray Diffraction (XRD)

The X-ray diffraction (XRD) study was carried out by powder X-ray diffractometer (Rigaku Miniflex with Cu Kα) in the angle 2θ range 20 - 80° at the rate of 2°/min to confirm the purity, crystallinity, dominated phase, and formation of compounds

Field Emission Scanning Electron Microscopy (FESEM)

To investigate the surface morphological behavior, **FESEM images** of sample has been recorded using the instrument **Carl Zeiss Sigma in the particle range of 1 μm at the magnification of 35 kX and applied voltage of 5 kV**

Thermoelectric Characterization

Electrical resistivity, thermal conductivity and Seebeck coefficient are calculated using **closed cycle refrigerator in the temperature range 10-350 K.**

Results & Discussions: Powder XRD Studies

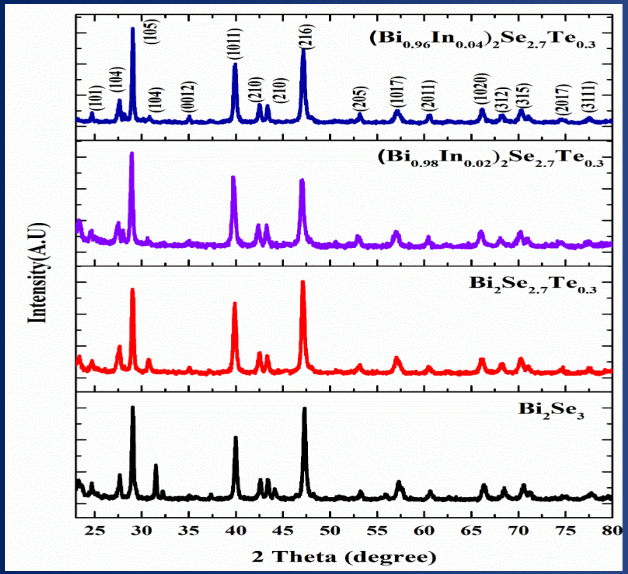


Fig. 1. XRD peak patterns of $(Bi_{1-x}In_x)_2Se_{2.7}Te_{0.3}$ samples

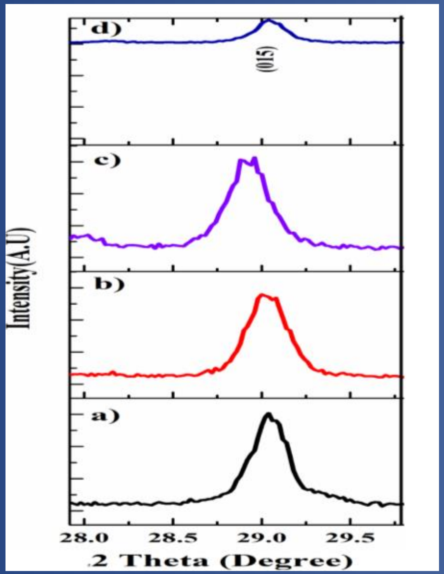


Fig. 2: Shifting of XRD Peak Patterns for the $(Bi_{1-x}In_x)_2Se_{2.7}Se_{0.3}$ samples

Table 1. XRD analysis data of $(Bi_{1-x}In_x)_2Se_{2.7}Te_{0.3}$ samples

Sample	R_p	R_{wp}	R_{ep}	χ^2	crystallite size(nm)	a = b Å	c Å	Lattice strain
Bi_2Se_3	5	11	8.3	2.0	48	4.13	28.6	0.0012
$Bi_2Se_{2.7}Te_{0.3}$	7	17	11	2.2	49	4.14	28.7	0.0017
$(Bi_{0.98}In_{0.02})_2Se_{2.7}Te_{0.3}$	10	17	13	1.7	85	4.15	28.8	0.0029
$(Bi_{0.96}In_{0.04})_2Se_{2.7}Te_{0.3}$	10	18	13	1.9	51	4.14	28.7	0.0028

Results & Discussions: FESEM Studies

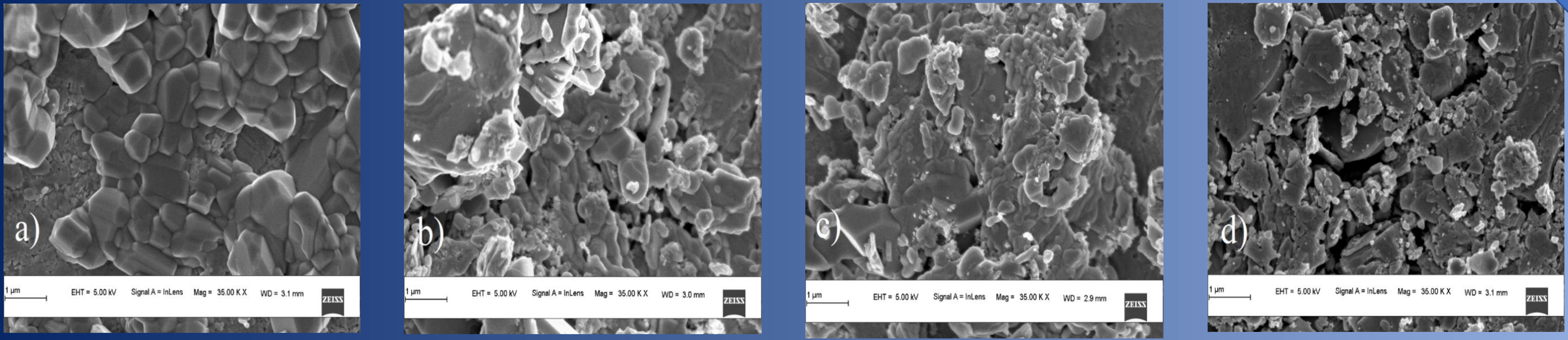


Fig. 3: FESEM images of samples

a) Bi_2Se_3 *b) $Bi_2Se_{2.7}Te_{0.3}$* *c) $(Bi_{0.98}In_{0.02})_2Se_{2.7}Te_{0.3}$* *d) $(Bi_{0.96}In_{0.04})_2Se_{2.7}Te_{0.3}$*

Results & Discussions: Electrical Resistivity & Seebeck coefficient Studies

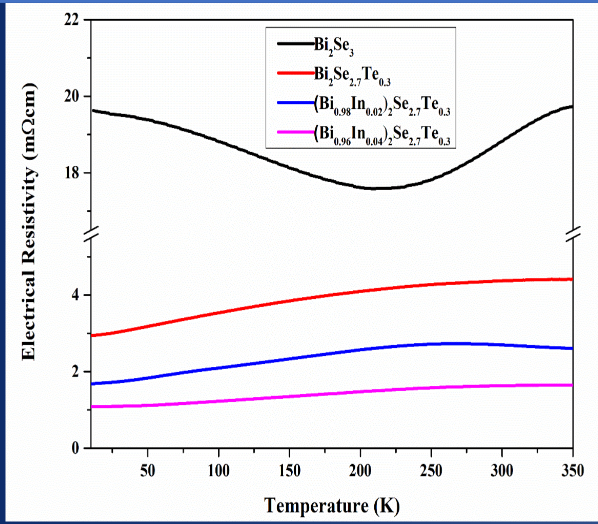


Fig. 4: Temperature dependent electrical resistivity of $(Bi_{1-x}In_x)_2Se_{2.7}Te_{0.3}$ samples

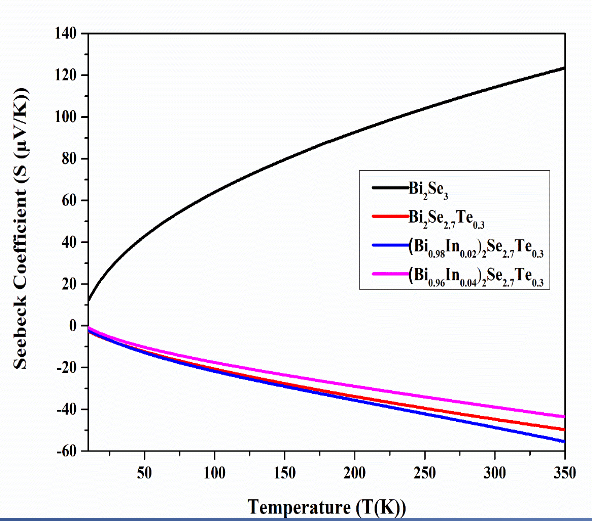


Fig. 5: Temperature-dependent Seebeck coefficient of $(Bi_{1-x}In_x)_2Se_{2.7}Te_{0.3}$ samples

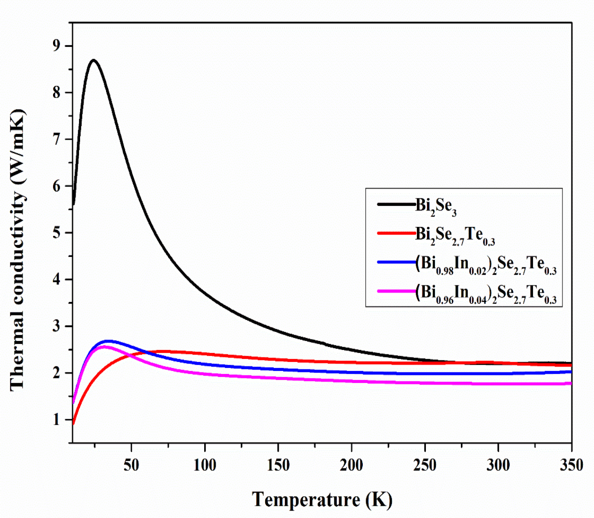


Fig. 6: Total thermal conductivity of $(Bi_{1-x}In_x)_2Se_{2.7}Te_{0.3}$ samples

Results & Discussions: Figure of Merit

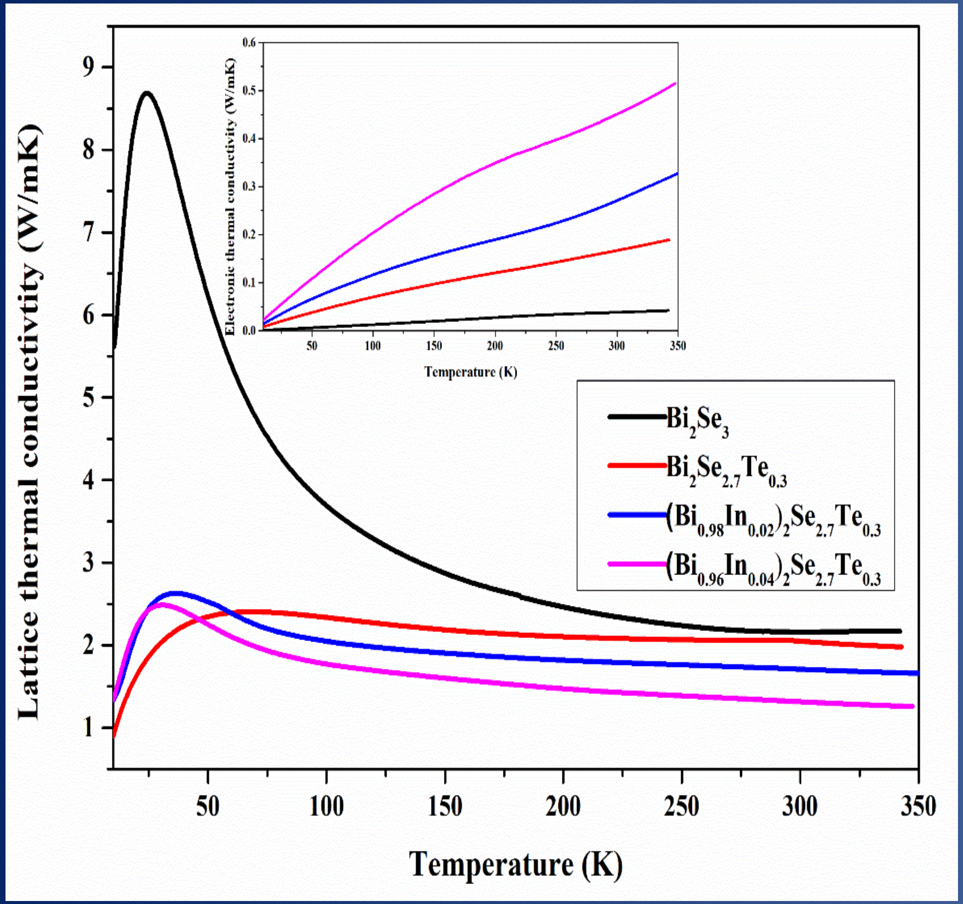


Fig. 7: Lattice thermal conductivity and electronic thermal conductivity of $(Bi_{1-x}In_x)_2Se_{2.7}Te_{0.3}$ samples

$$K_e = \frac{L_0 T}{\rho}$$

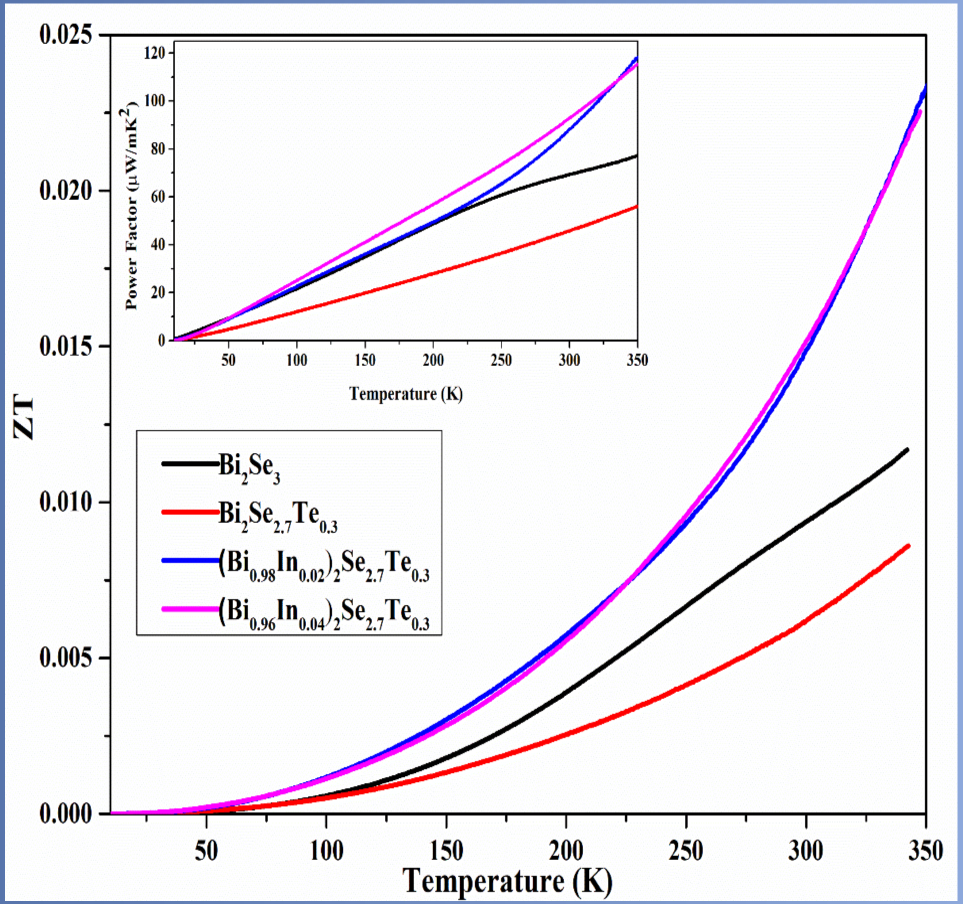


Fig. 8: Temperature-dependent Power factor and ZT value of $(Bi_{1-x}In_x)_2Se_{2.7}Te_{0.3}$ samples

$$PF = \frac{S^2}{\rho}$$

$$ZT = \frac{S^2 T}{K\rho}$$

Conclusion

- The sample $(Bi_{0.96}In_{0.04})_2Se_{2.7}Te_{0.3}$ shows a 9 times reduction in electrical resistivity compared to the pristine sample.
- At low temperature, the thermal conductivity was found to reduce by 7.5 times for $(Bi_{0.96}In_{0.04})_2Se_{2.7}Te_{0.3}$ in comparison with the pristine sample.
- The highest *ZT* values are found to be 0.023 and 0.022 for $(Bi_{0.98}In_{0.02})_2Se_{2.7}Te_{0.3}$, $(Bi_{0.96}In_{0.04})_2Se_{2.7}Te_{0.3}$ respectively, with a *PF* value of about 120 μW/mK^2 at 350 K. From the present study, it is realized that co-doping reduces thermal conductivity and electrical resistivity.

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