# Supplemental material for "Transport phenomena of TiCoSb: Defects induced modification in structure and density of states"

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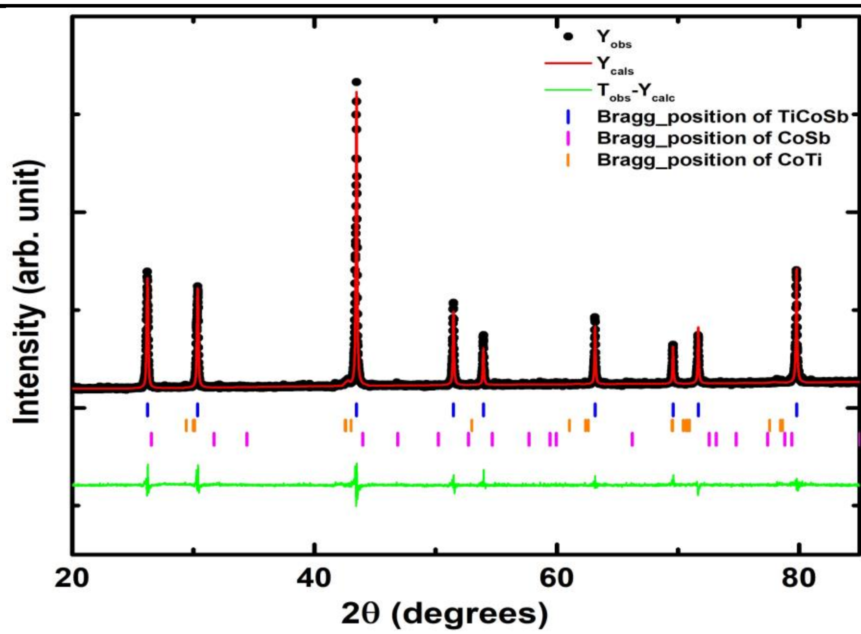
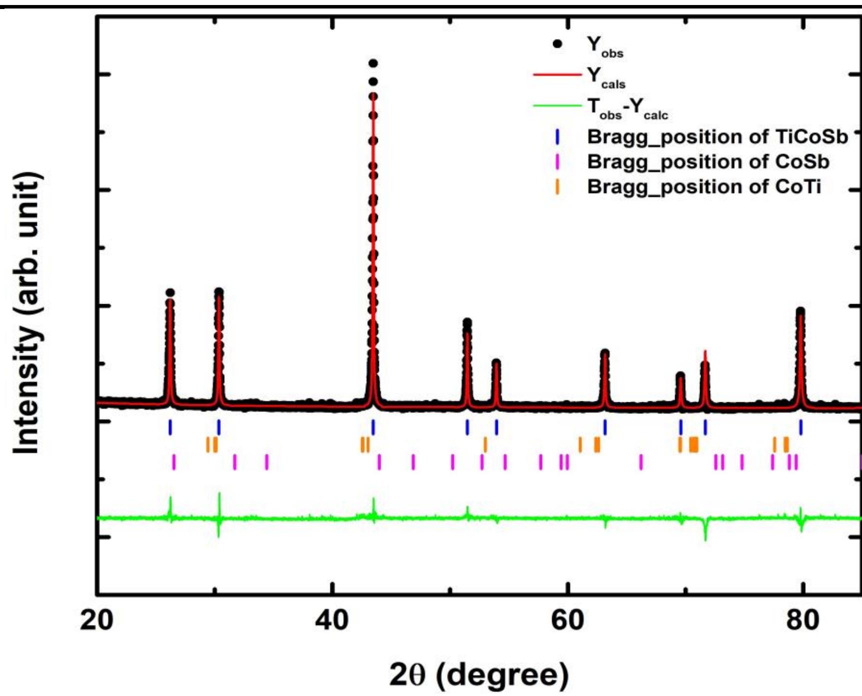
**FIGURE S1:** (Color online). X-ray diffraction patterns after Rietveld refinement and the corresponding refinement parameters have been obtained, using FullProf software for $TiCoSb_{1+x}$ (x = 0.00, 0.01, 0.02, 0.03, 0.04, 0.06) samples at room temperature.

(a)

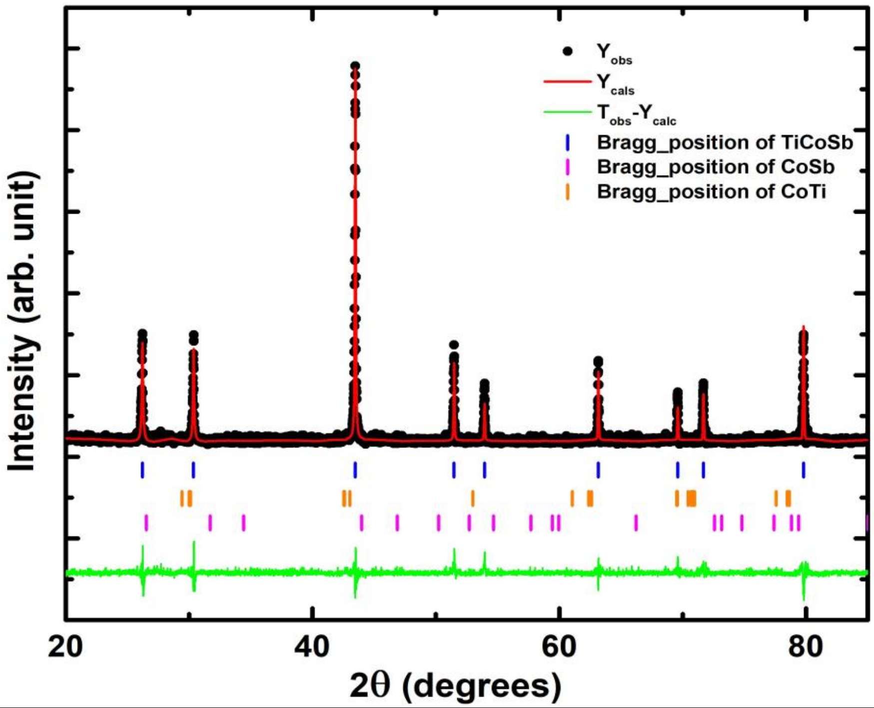



| Phase | RT<br>TiCoSb |
|---|---|
| Cell (Å) | *a* =b= *c*: 5.8841 |
| *Site occupancy: Ti/Co/Sb* | 1/1.002/1 |
| $B_{iso}$ (Å$^2$) | 0.53 |
| *TiCoSb Phase (%)* | 97.4 |
| *CoSb Phase (%)* | 0.1 |
| *TiCo Phase (%)* | 2.5 |
| $R_p$ (%) | 21.4 |
| $R_{wp}$(%) | 18.4 |
| $R_{exp}$(%) | 10.512 |
| Gof | 3.04 |

(b)

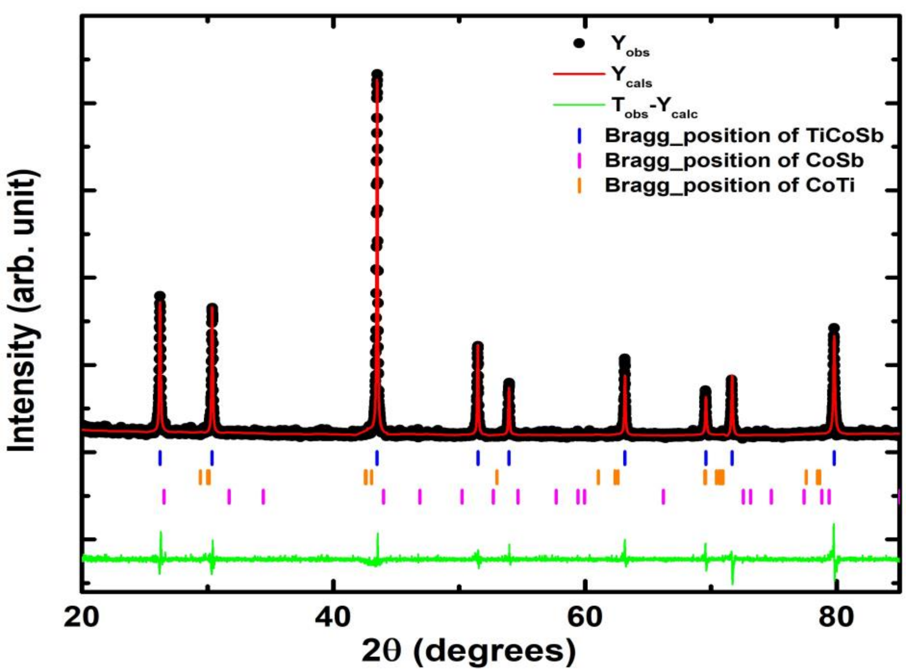



| Phase | RT<br>$TiCoSb_{1.01}$ |
|---|---|
| Cell (Å) | *a* =b= *c*: 5.88396 |
| *Site occupancy: Ti/Co/Sb* | 1/0.992/1 |
| $B_{iso}$ (Å$^2$) | 0.57 |
| *TiCoSb Phase (%)* | 98.49 |
| *CoSb Phase (%)* | 0.27 |
| *TiCo Phase (%)* | 1.24 |
| $R_p$ (%) | 18.46 |
| $R_{wp}$(%) | 15.91 |
| $R_{exp}$(%) | 9.72 |
| Gof | 2.68 |



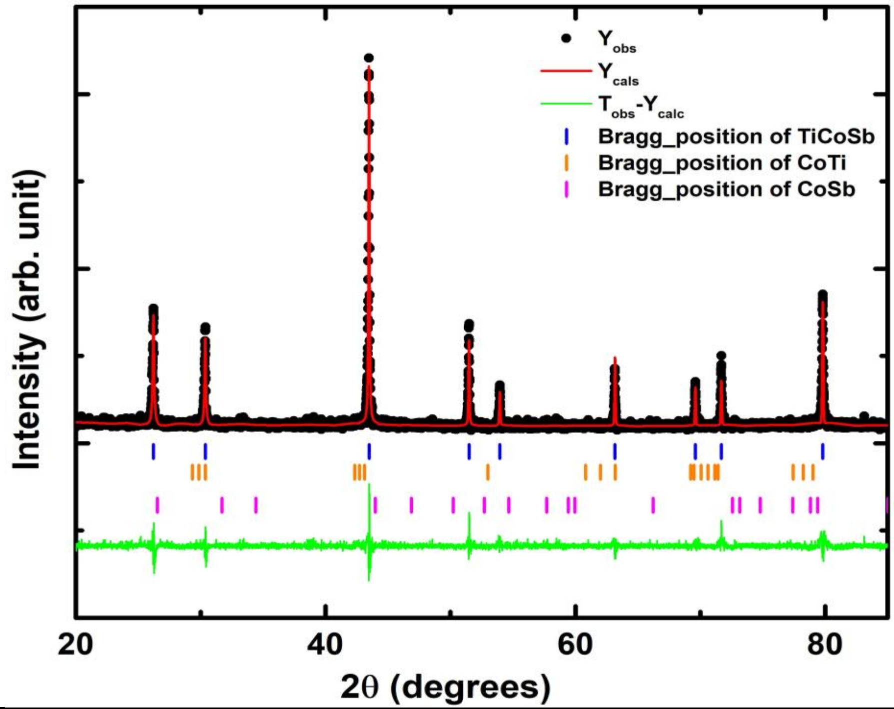

| Phase | RT<br>$TiCoSb_{1.02}$ |
|---|---|
| Cell (Å) | *a* =b= *c*:5.88356 |
| *Site occupancy: Ti/Co/Sb* | 1/0.988/1 |
| $B_{iso}$ (Å$^2$) | 0.68 |
| *TiCoSb Phase (%)* | 98.76 |
| *CoSb Phase (%)* | 0.52 |
| *TiCo Phase (%)* | 0.72 |
| $R_p$ (%) | 20.61 |
| $R_{wp}$(%) | 16.36 |
| $R_{exp}$(%) | 13.06 |
| Gof | 1.74 |

(e)



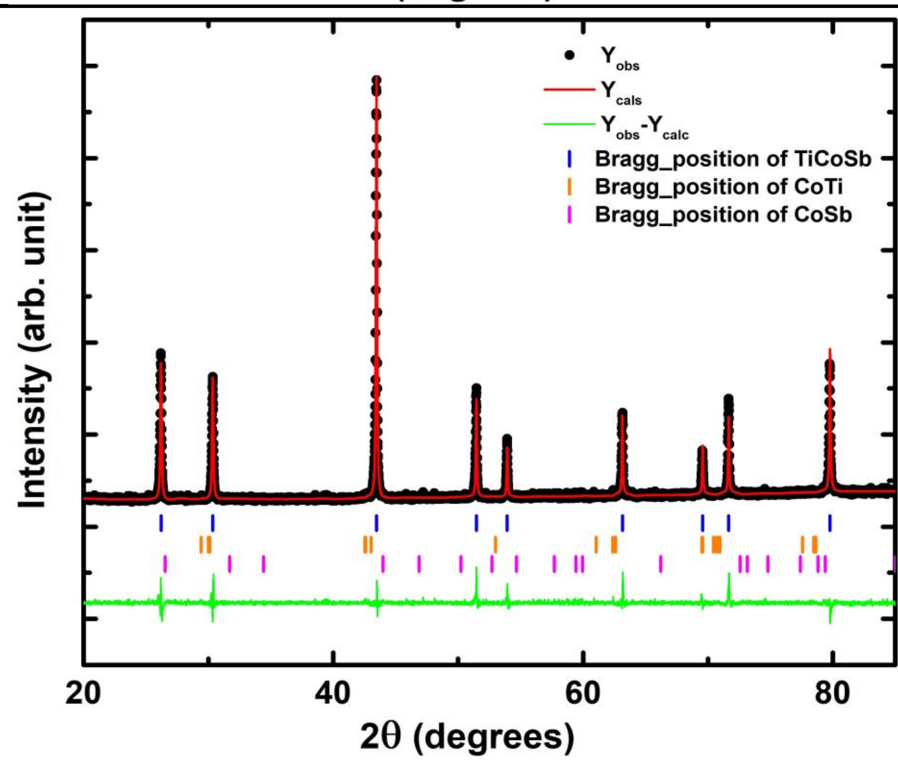

| Phase | RT<br>$TiCoSb_{1.03}$ |
|---|---|
| Cell (Å) | *a* =b= *c*: 5.88308 |
| *Site occupancy: Ti/Co/Sb* | 1/0.983/1 |
| $B_{iso}$ (Å$^2$) | 0.52 |
| *TiCoSb Phase (%)* | 98.63 |
| *CoSb Phase (%)* | 0.77 |
| *TiCo Phase (%)* | 0.6 |
| $R_p$ (%) | 22.574 |
| $R_{wp}$(%) | 19.854 |
| $R_{exp}$(%) | 14.26 |
| Gof | 1.94 |

(a)



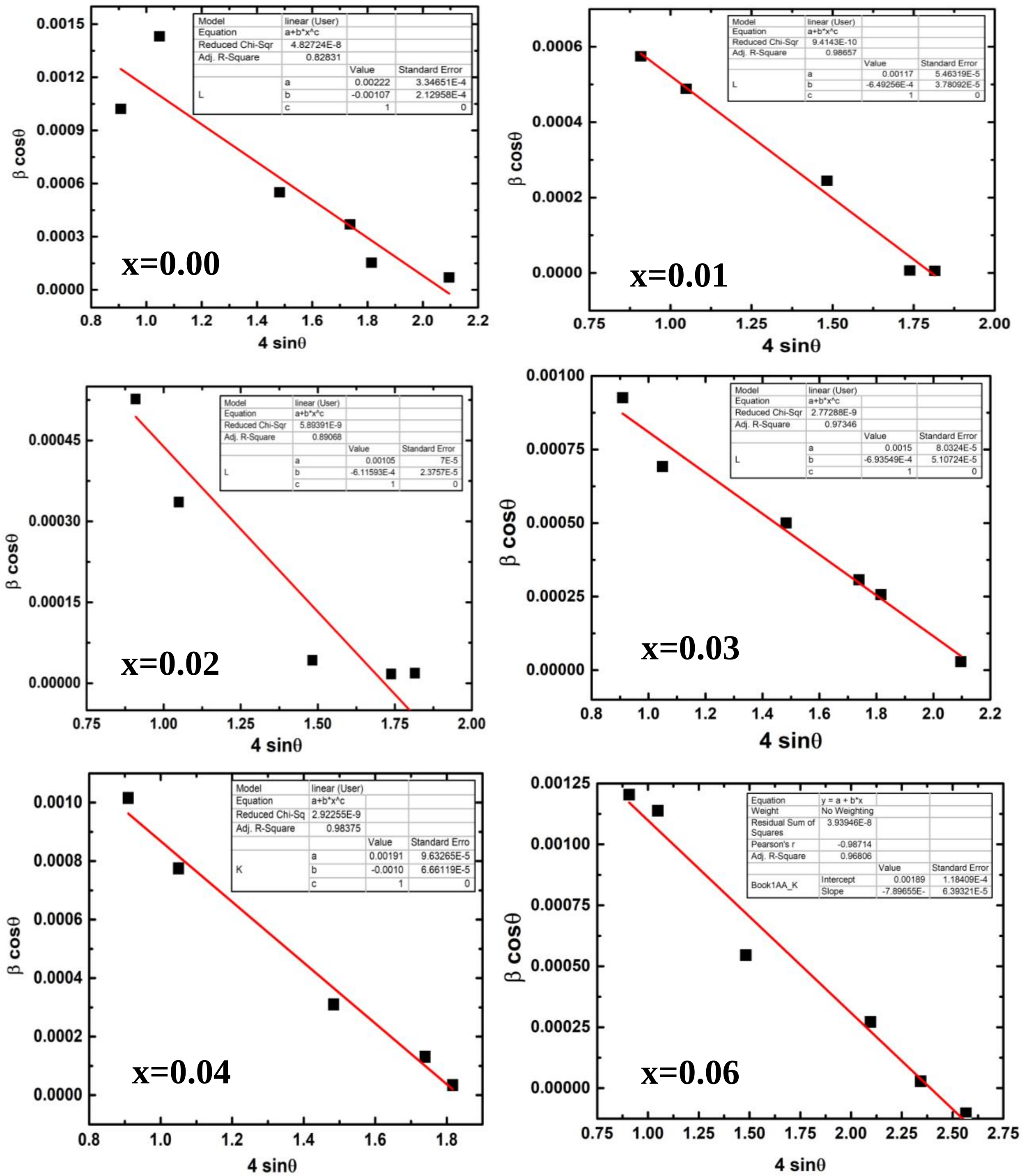

| Phase | RT |
|---|---|
| | $TiCoSb_{1.04}$ |
| Cell (Å) | *a* =b= *c*: 5.88246 |
| *Site occupancy: Ti/Co/Sb* | 1/0.975/1 |
| $B_{iso}$ (Å$^2$) | 0.37 |
| *TiCoSb Phase (%)* | 97.94 |
| *CoSb Phase (%)* | 1.5 |
| *TiCo Phase (%)* | 0.56 |
| $R_p$ (%) | 23.34 |
| $R_{wp}$(%) | 17.38 |
| $R_{exp}$(%) | 11.30 |
| Gof | 2.36 |

(b)




| Phase | RT |
|---|---|
| | $TiCoSb_{1.06}$ |
| Cell (Å) | *a* =b= *c*: 5.88434 |
| *Site occupancy: Ti/Co/Sb* | 1/0.972/1 |
| $B_{iso}$ (Å$^2$) | 0.44 |
| *TiCoSb Phase (%)* | 96.4 |
| *CoSb Phase (%)* | 3.4 |
| *TiCo Phase (%)* | 0.2 |
| $R_p$ (%) | 25.08 |
| $R_{wp}$(%) | 21.84 |
| $R_{exp}$(%) | 12.62 |
| Gof | 3 |

**FIGURE S2:** (Color online). Williamson-Hall plot of polycrystalline $TiCoSb_{1+x}$ (x=0.0, 0.01, 0.02, 0.03, 0.04, 0.06) HH materials. Solid line represents best linear fit.



## Calculation of Dislocation density ($N_D$) using modified Williamson-Hall plot:

Dislocation density ($N_D$) of the samples has been obtained using the following equation:

$$\Delta K = \frac{0.9}{d} + \frac{\pi A^2 B_D^2}{2} N_D^{1/2} K^2 C \pm O(K^4 C^2)$$

$C$ = Average dislocation contrast factor = $C_{h00} \frac{1 - q(h^2k^2 + k^2l^2 + h^2l^2)}{(h^2+k^2+l^2)^2}$.

$h, k, l$ **:** Indices of crystal plane
$C_{h00}$ **:** Average dislocation contrast factor corresponding to the *h00* reflection.
$q$ **:** Constant parameter = -2.7 [1]
$A$ **:** Parameter related to the effective outer cut-off radius of dislocations
$B_D$ **:** Burgers vector
$d$ **:** Average crystallite size

It is assumed that the parameters q, $A$ and $B_D$ do not change significantly for samples $TiCoSb_{1+x}$ (x=0, 0.01, 0.02, 0.03, 0.04, 0.06). Here, we have estimated relative dislocation densities $N_D / N_{D|x=0}$ to avoid the constant terms.

$$\left(\frac{N_D}{N_{D|=0}}\right) = \left(\frac{m_x}{m_{x=0}}\right)^2.$$

Where $m_x$ is the slope *'ΔK versus $K^2C$'* curve, estimated for each sample $TiCoSb_{1+x}$ (x=0.0, 0.01, 0.02, 0.3, 0.04, 0.06). And $m_{x=0}$ represents the slope of *'ΔK versus $K^2C$'* curve for x = 0.

**FIGURE S3:** (Color online). Modified Williamson-Hall plot of polycrystalline $TiCoSb_{1+x}$ (x=0.0, 0.01, 0.02, 0.03, 0.04, 0.06) HH materials. Solid line represents best linear fit.

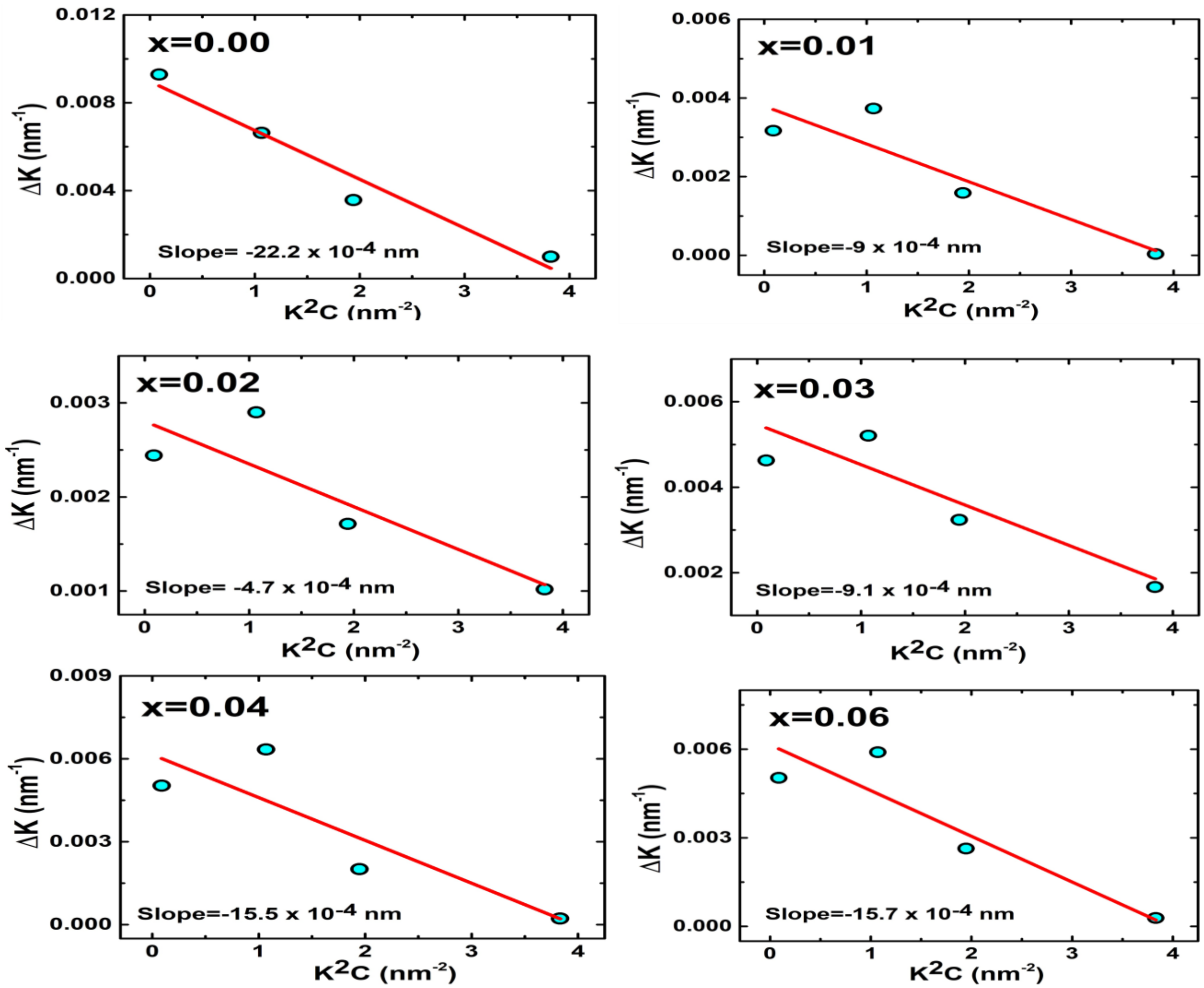
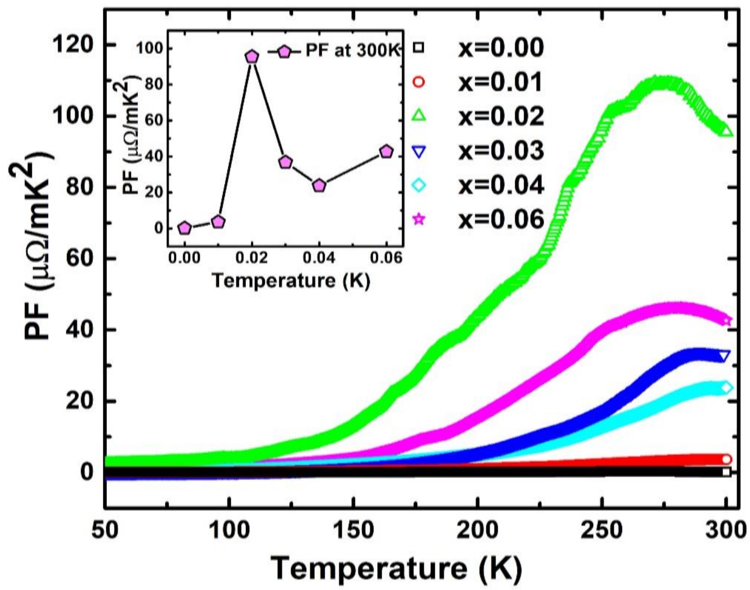


**FIGURE S4: (Color online).** Variation of PF with temperature of polycrystalline $TiCoSb_{1+x}$ (x=0.0, 0.01, 0.02, 0.03, 0.04, 0.06) HH materials. Inset depicts Sb concentration dependent PF at room temperature (300 K).




## Reference:

[1] T. Ungár, S. Ott, P. G. Sanders, A. Borbély, and J. R. Weertman, Acta Mater. **46**, 3693 (1998).