

SUPPLEMENTARY INFORMATION

Structural Evolution from Neutron Powder Diffraction of Nanostructured SnTe Obtained by Arc Melting

Javier Gainza ^{1,*}, Federico Serrano-Sánchez ¹, João E. F. S. Rodrigues ^{1,2}, Oscar J. Dura ³, Brenda Fragoso ⁴, Mateus M. Ferrer ⁴, Norbert M. Nemes ⁵, José L. Martínez ¹, María T. Fernández-Díaz ⁶ and José A. Alonso ^{1,*}

¹ Instituto de Ciencia de Materiales de Madrid (ICMM), Consejo Superior de Investigaciones Científicas (CSIC), Sor Juana Inés de la Cruz 3, 28049 Madrid, Spain

² European Synchrotron Radiation Facility (ESRF), 71 Avenue des Martyrs, 38000 Grenoble, France

³ E.T.S. Ingeniería Industrial (ETSII), Instituto Regional de Investigación Científica Aplicada (IRICA), Universidad de Castilla-La Mancha (UCLM), 13071 Ciudad Real, Spain

⁴ CCAF, PPGCEM/CDTec, Federal University of Pelotas, Pelotas 96010-610, RS, Brazil

⁵ Departamento de Física de Materiales, Universidad Complutense de Madrid, 28040 Madrid, Spain

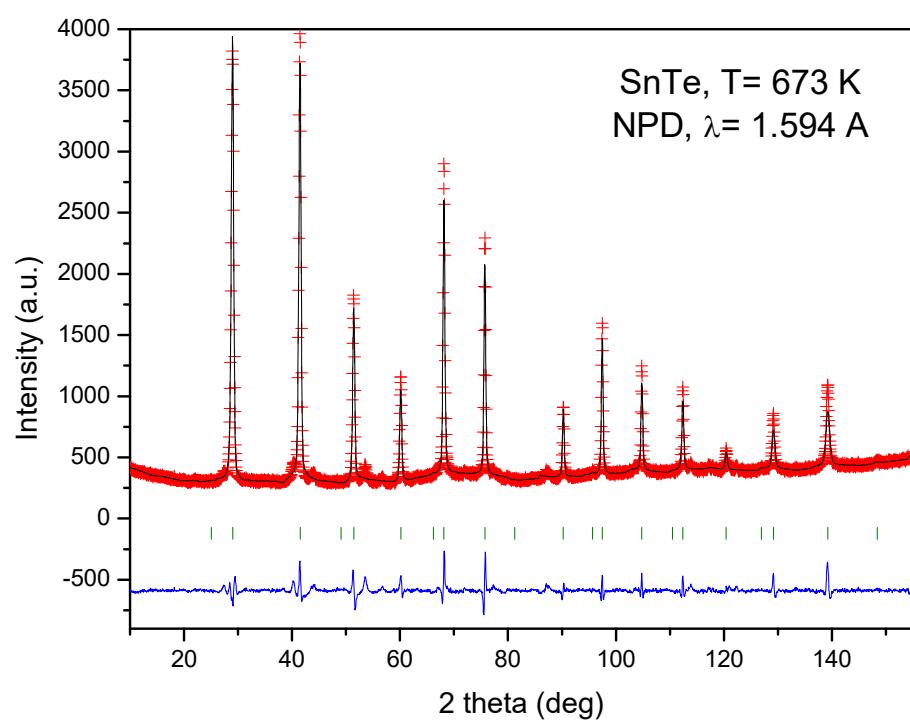
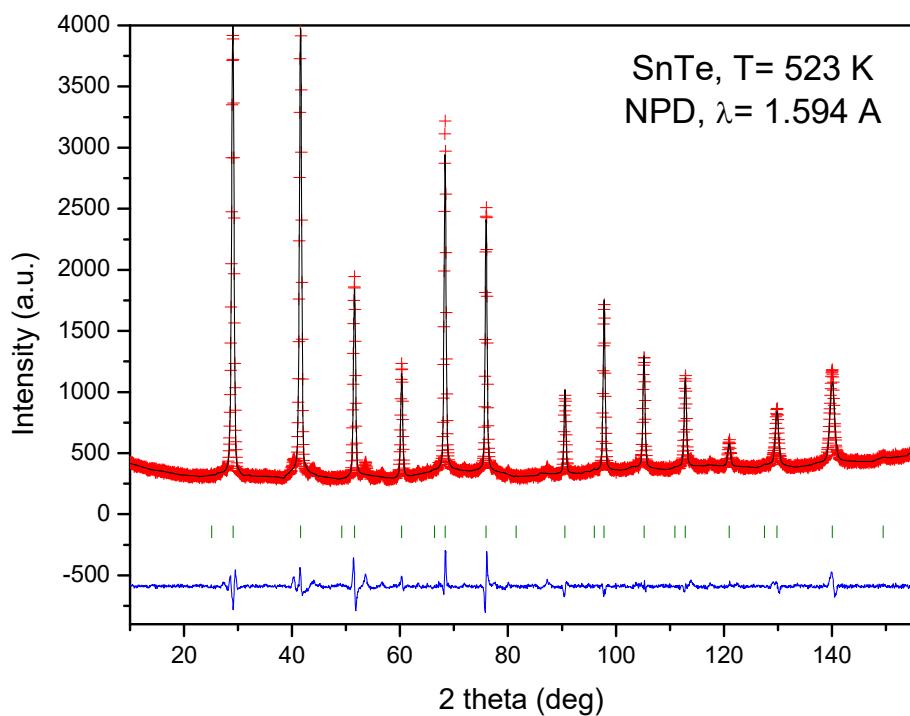
⁶ Institut Laue Langevin, BP 156X, 38042 Grenoble, France

* Correspondence: j.gainza@csic.es (J.G.); ja.alonso@icmm.csic.es (J.A.A.)

Table S1. Main structural parameters after the Rietveld refinement from NPD data at 973 K for SnTe, defined in the cubic *Fm-3m* space group; $a = 6.4042(3)$ Å.

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>B</i> (Å ²)	<i>f_{occ}</i>
Sn	4 <i>a</i>	0.0	0.0	0.0	4.8(2)	0.97(5)
Te	4 <i>b</i>	0.5	0.5	0.5	5.5(3)	1.0

Discrepancy factors: $R_p = 3.36\%$, $R_{wp} = 4.90\%$, $R_{Bragg} = 3.06\%$; $\chi^2 = 5.58$



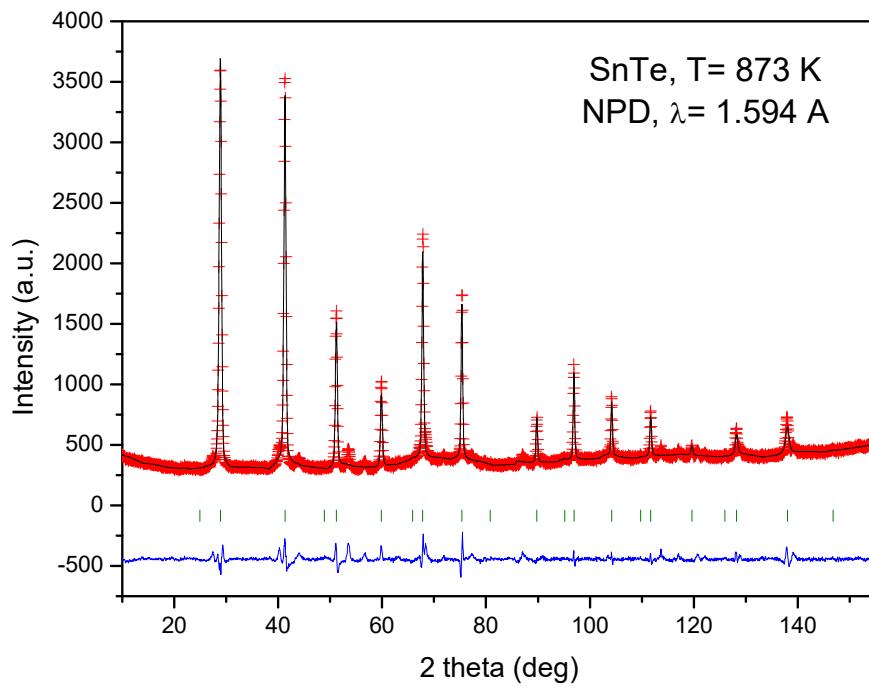
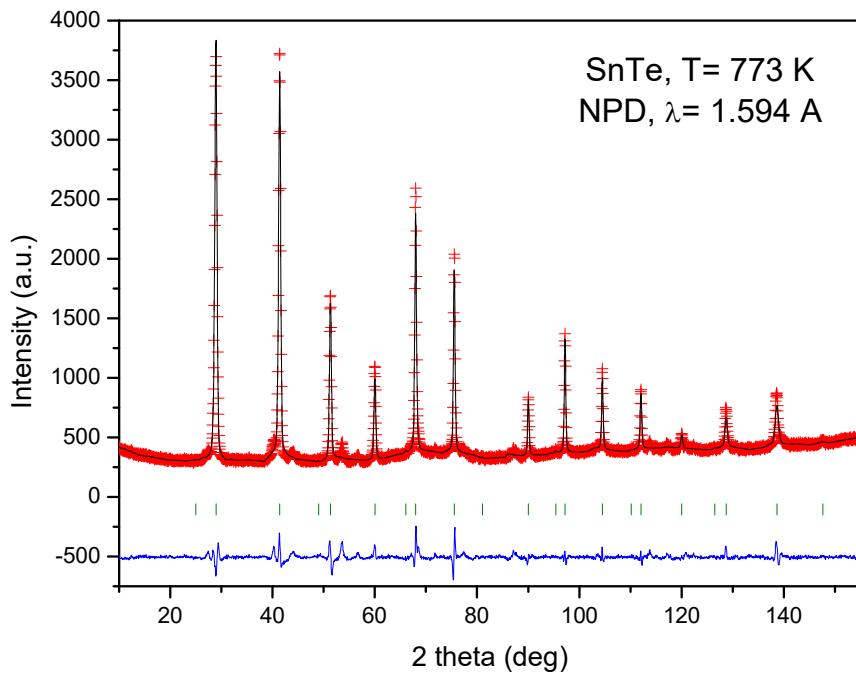


Figure S1. NPD profiles after the Rietveld refinement of the cubic crystal structure at 523, 673, 773 and 873 K.

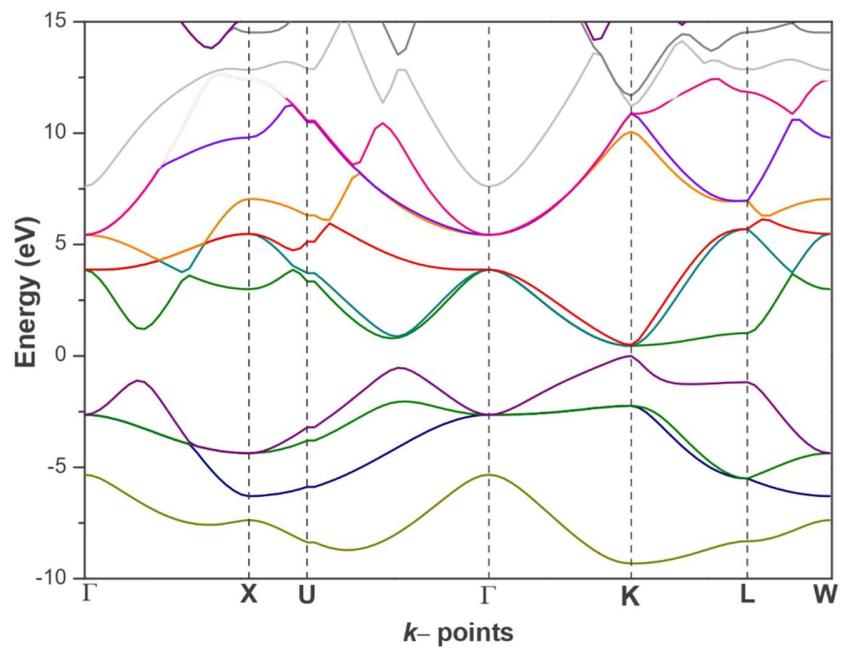


Figure S2. Band structure of the SnTe model.

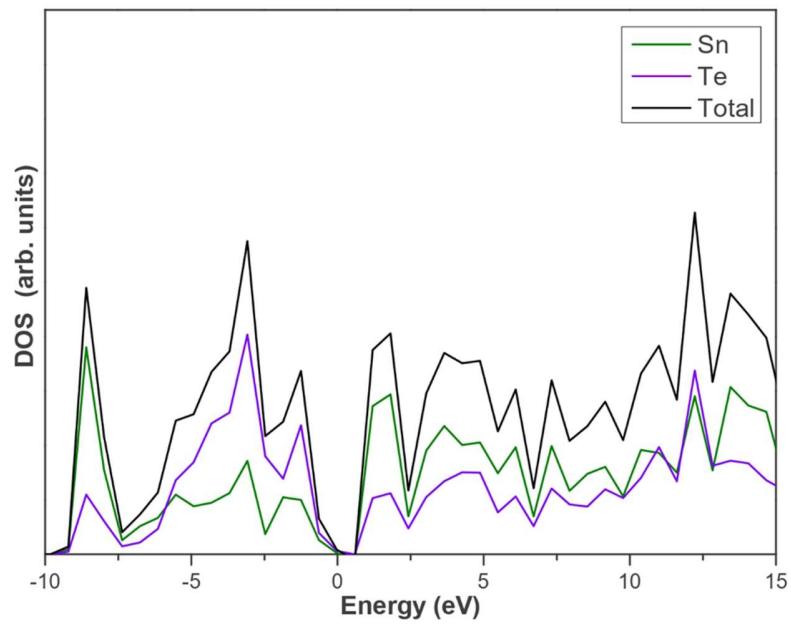


Figure S3. Density of States of the SnTe model.

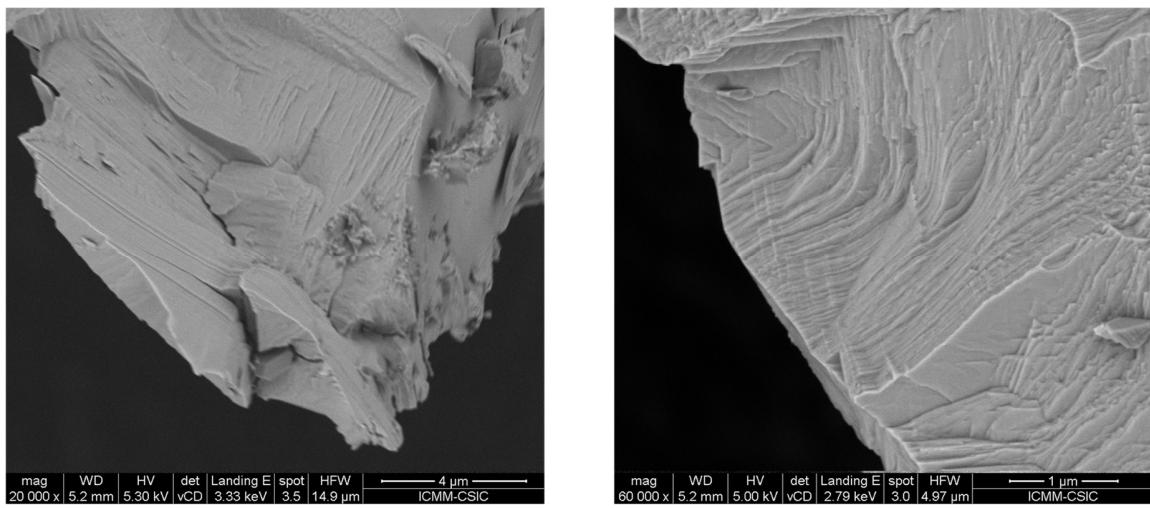


Figure S4. SEM images with (a) 20,000x and (b) 60,000x magnification, illustrating the nanostructuration in layers observed in SnTe prepared by arc melting.

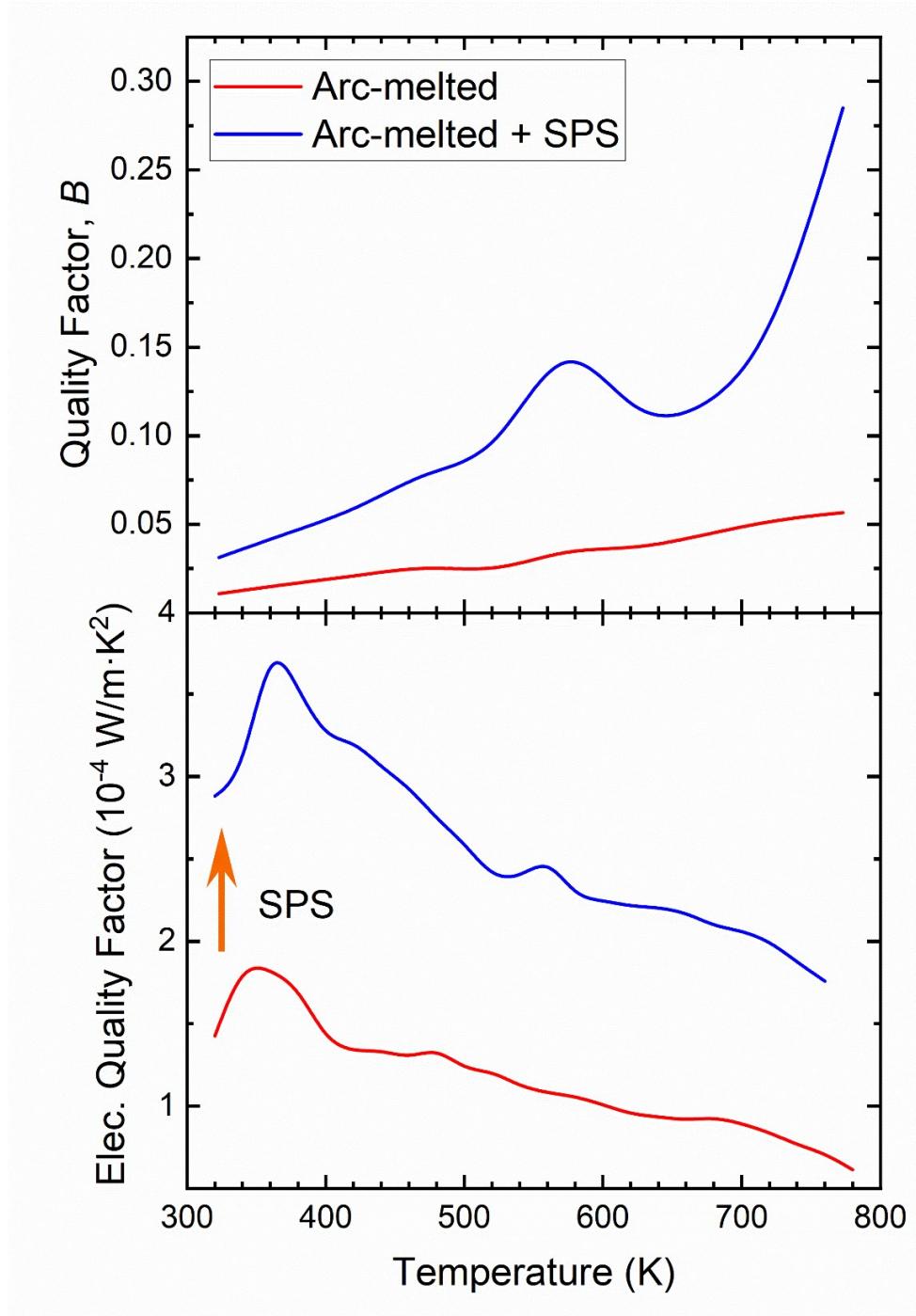


Figure S5. (a) Quality Factor, B , and (b) electronic Quality Factor, B_E , of the arc-melted SnTe and the arc-melted and sintered SnTe.

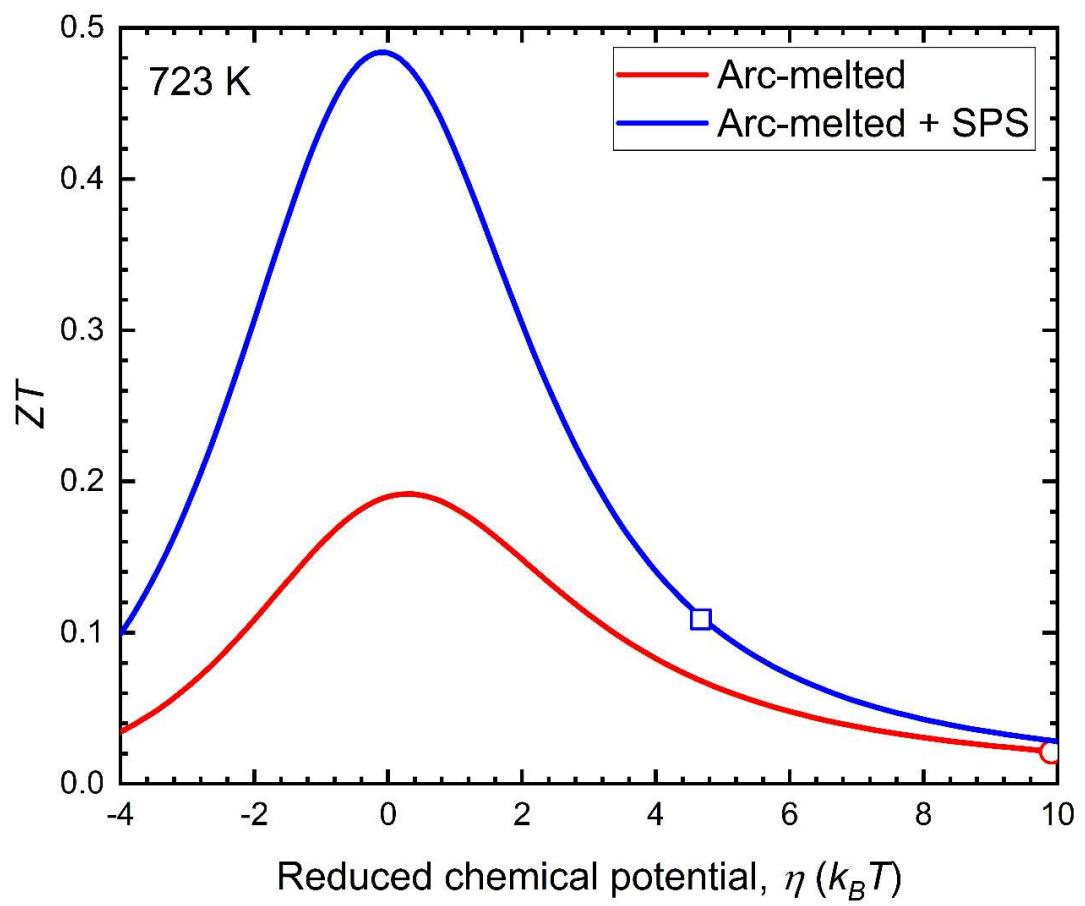


Figure S6. ZT vs reduced Fermi energy (η) relation. The line is the calculated data, and the point is the experimental measurement.