Supporting Information

Comparative Thermoelectric Properties of Polypropylene Composites Melt-Processed Using Pyrograf® III Carbon Nanofibers

Antonio J. Paleo [1,*], Beate Krause [2], Ana R. Mendes [3], Carlos J. Tavares [4], Maria F. Cerqueira [5,6], Enrique Muñoz [7] and Petra Pötschke [2]

[1] 2C2T-Centre for Textile Science and Technology, University of Minho, Campus de Azurém,
4800-058 Guimarães, Portugal
[2] Leibniz-Institut für Polymerforschung Dresden e.V. (IPF), Hohe Str. 6, 01069 Dresden, Germany;
krause-beate@ipfdd.de (B.K.); poe@ipfdd.de (P.P.)
[3] SEMAT/UM-Materials Characterization Services, University of Minho, 4804-533 Guimarães, Portugal; a85605@alunos.uminho.pt
[4] Physics Centre of Minho and Porto Universities (CF-UM-PT), University of Minho,
4804-533 Guimarães, Portugal; ctavares@fisica.uminho.pt
[5] INL—International Iberian Nanotechnology Laboratory, Av. Mestre, Jose Veiga, 4715-330 Braga, Portugal; fcerqueira@fisica.uminho.pt
[6] CFUM—Center of Physics of the University of Minho, Campus de Gualtar, 4710-057 Braga, Portugal
[7] Facultad de Física, Pontificia Universidad Católica de Chile, Santiago 7820436, Chile; munoztavera@gmail.com
* Correspondence: ajpaleovieito@2c2t.uminho.pt

2.1 Materials and their Processing

Figure S1. Photos showing the steps of manufacturing the samples: from let to right: extruded starnd, pelletized material, compression molded plate, strip cut from the plate and used for the preparation of the sample for TE measurements.

2.5 Thermoelectric analysis

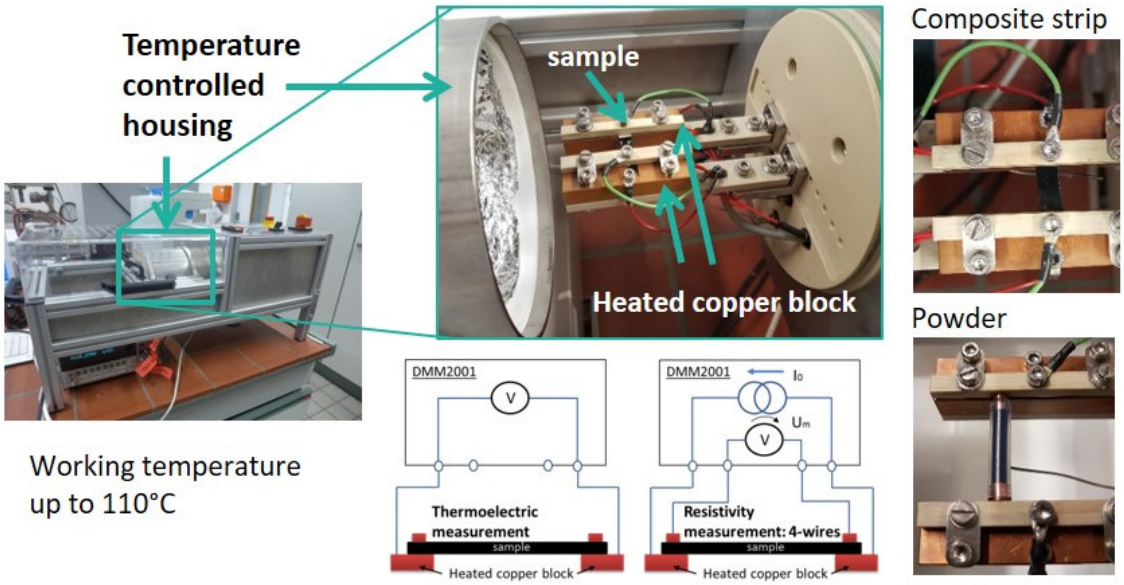

Figure S2. Photos and schema of the used thermoelectric measurement equipment used to measure Seebeck coefficeint and electrical conductivity simultaneously (replotted from [1]).

3.2 XRD and Raman analysis

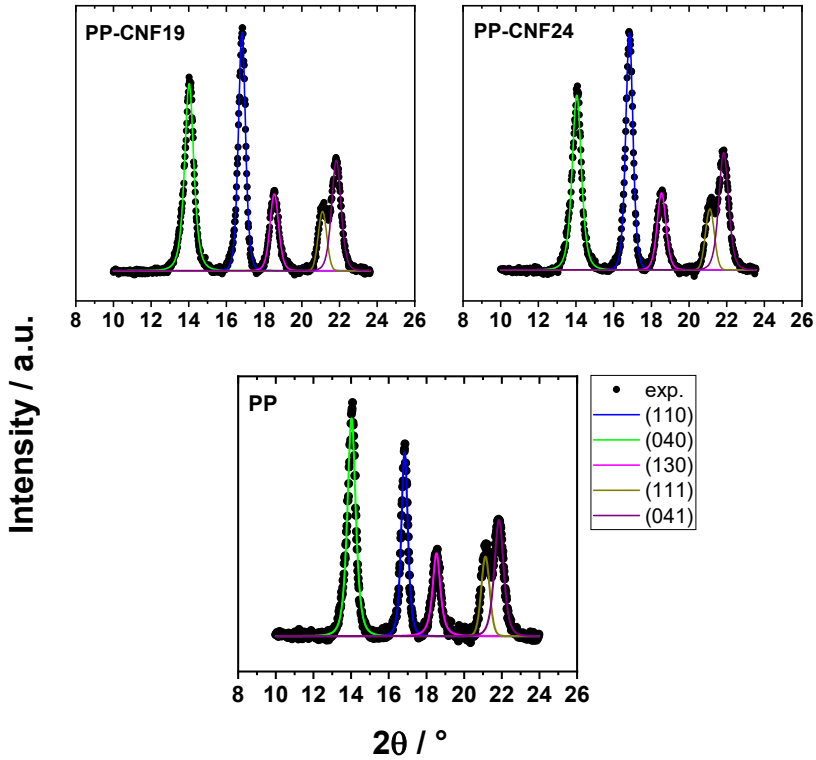

Figure S3. Experimental and fitted X-ray diffraction patterns for polypropylene and the matrix of this material in the PP/CNF composites.

Table S1. Parameters from the fitted X-ray diffraction peaks (hkl) in Figure S1. For each peak, the respective 2θ (°) position, FWHM (°) and crystalline domain, D, (nm) size are presented.

Sample	(110)	(040)	(130)	(111)	(041)
	2θ (°) / FWHM (°) / D (nm)	2θ (°) / FWHM (°) / D (nm)	2θ (°) / FWHM (°) / D (nm)	2θ (°) / FWHM (°) / D (nm)	2θ (°) / FWHM (°) / D (nm)
PP	14.02	16.84	18.53	21.13	21.85
	0.51	0.40	0.48	0.52	0.58
	15.7	20.1	16.8	15.6	14.0
PP-CNF19	14.02	16.82	18.54	21.10	21.83
	0.56	0.44	0.54	0.53	0.58
	15.4	18.3	14.9	15.3	14.0
PP-CNF24	14.04	16.83	18.54	21.11	21.84
	0.57	0.45	0.55	0.55	0.61
	14.1	17.9	14.6	14.7	13.3

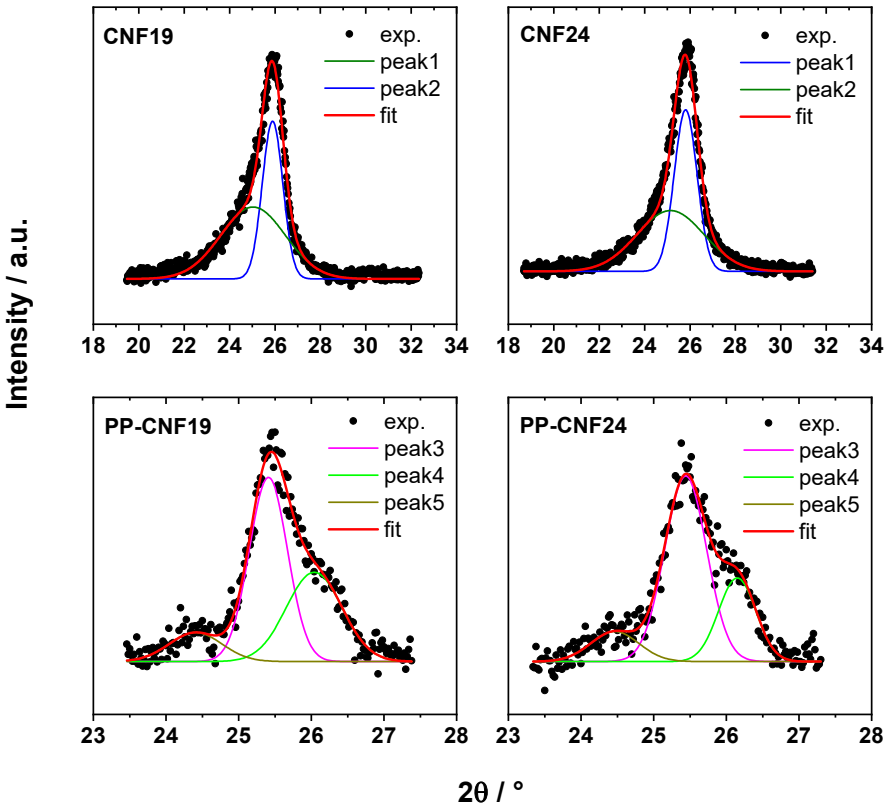

Figure S4. Experimental and fitted X-ray diffraction patterns in the region of the main graphitic contribution for the CNF and PP/CNF composites.

Table S2. Parameters from the fitted X-ray diffraction peaks in Figure S2. For each peak, the respective 2θ (°) position, FWHM (°) and crystalline domain, D, (nm) size are presented.

Sample	Peak 1 2θ (°) / FWHM (°) / D (nm)	Peak 2 2θ (°) / FWHM (°) / D (nm)	Peak 3 2θ (°) / FWHM (°) / D (nm)	Peak 4 2θ (°) / FWHM (°) / D (nm)	Peak 5 2θ (°) / FWHM (°) / D (nm)
CNF19	25.03 3.36 2.4	25.89 1.07 7.6	-	-	-
CNF24	25.14 3.48 2.3	25.81 1.18 6.9	-	-	-
PP-CNF19	-	-	24.41 0.85 9.6	25.41 0.62 13.1	26.04 0.90 9.1
PP-CNF24	-	-	24.46	25.44	26.15

	0.78	0.68	0.60
	10.4	12.0	13.6

3.5 Thermoelectric analysis of PP/CNF composites from 40 °C to 100 °C

Table S3. Electrical volume conductivity and Seebeck coefficient of CNFs and PP/CNF composites from 40 °C to 100 °C. (Data for CNF19 and PP/CNF19 taken with permission from ref. [2]. Data of CNF 24 taken with permission from ref. [3]).

T (°C)	Sample	Conductivity (S/m)	Seebeck (µV/K)	Power Factor (µW/mK^2)	zT
40	CNF19	131.5 ± 20	−5.4 ± 0.2	3.8×10^{-3}	-
	CNF24	131.6 ± 0.1	−5.4 ± 0.1	3.8×10^{-3}	-
60	CNF19	131.5 ± 19	−5.6 ± 0.1	4.1×10^{-3}	-
	CNF24	129.2 ± 10	−5.4 ± 0.1	3.8×10^{-3}	-
80	CNF19	131.2 ± 17	−5.6 ± 0.1	4.1×10^{-3}	-
	CNF24	124.4 ± 13	−5.8 ± 0.1	4.2×10^{-3}	-
100	CNF19	127.0 ± 14	−5.8 ± 0.1	4.3×10^{-3}	-
	CNF24	123.9 ± 14	−5.9 ± 0.1	4.3×10^{-3}	-
40	PP/CNF19	16.5 ± 0.7	−3.8 ± 0.1	2.4×10^{-4}	3.0×10^{-7}
	PP/CNF24	62.7 ± 7	−4.4 ± 0.1	1.2×10^{-3}	1.3×10^{-6}
60	PP/CNF19	16.1 ± 0.7	−4.0 ± 0.1	2.6×10^{-4}	3.6×10^{-7}
	PP/CNF24	56.0 ± 2	−5.1 ± 0.2	1.5×10^{-3}	1.6×10^{-6}
80	PP/CNF19	15.3 ± 0.6	−4.2 ± 0.1	2.7×10^{-4}	4.0×10^{-7}
	PP/CNF24	56.8 ± 2	−5.5 ± 0.1	1.7×10^{-3}	2.0×10^{-6}
100	PP/CNF19	13.9 ± 0.4	−4.3 ± 0.1	2.6×10^{-4}	4.4×10^{-7}
	PP/CNF24	53.2 ± 0.1	−6.1 ± 0.1	2.0×10^{-3}	2.5×10^{-6}

References:

1. Krause, B.; Pötschke, P. Polyethylene Glycol as Additive to Achieve N-Conductive Melt-Mixed Polymer/Carbon Nanotube Composites for Thermoelectric Application. *Nanomaterials* **2022**, *12*, 3812.
2. Paleo, A.J.; Krause, B.; Cerqueira, M.F.; Muñoz, E.; Pötschke, P.; Rocha, A.M. Nonlinear Thermopower Behaviour of N-Type Carbon Nanofibres and Their Melt Mixed Polypropylene Composites. *Polymers* **2022**, *14*, 269.
3. Paleo, A.J.; Krause, B.; Cerqueira, M.F.; Muñoz, E.; Pötschke, P.; Rocha, A.M. Electronic Features of Cotton Fabric e-Textiles Prepared with Aqueous Carbon Nanofiber Inks. *ACS Applied Engineering Materials* **2023**, *1*, 122-131, doi:10.1021/acsaenm.2c00023.