

Supporting information to

Influence of polyvinylpyrrolidone on thermoelectric properties of melt-mixed polymer/carbon nanotube composites

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Table S1. TE properties of PC composites with SWCNT and PVP in different quantities (electrical volume conductivity, Seebeck coefficient, power factor, figure of merit ZT) measured at 40°C

| Composite | Vol. conductivity σ (S/m) | Seebeck coeff. S ($\mu\text{V/K}$) | Power factor PF ($\mu\text{W}/(\text{m}\cdot\text{K}^2)$) | ZT* (-) |
|----------------------------------|-------------------------------------|---|--|----------------------|
| PC/ 0.75 wt% SWCNT [1] | 0.9 | 39.5 ± 0.8 | 1.4×10^{-3} | 1.5×10^{-6} |
| PC/ 0.75 wt% SWCNT + 1.5 wt% PVP | 0.2 ± 0.0 | 14.0 ± 0.9 | 4.6×10^{-5} | 4.8×10^{-8} |
| PC/ 1 wt% SWCNT [1] | 1.0 | 36.7 ± 2.0 | 1.3×10^{-3} | 1.4×10^{-6} |
| PC/ 1 wt% SWCNT + 2 wt% PVP | 0.5 ± 0.0 | 9.1 ± 0.7 | 4.0×10^{-5} | 4.2×10^{-8} |
| PC/ 2 wt% SWCNT [1] | 1.0 | 37.8 ± 0.3 | 1.2×10^{-3} | 1.5×10^{-6} |
| '' + 2 wt% PVP | 1.9 ± 0.0 | -19.6 ± 2.6 | 7.3×10^{-4} | 7.7×10^{-7} |
| '' + 3 wt% PVP | 2.3 ± 0.0 | -30.6 ± 0.4 | 2.2×10^{-3} | 2.3×10^{-6} |
| '' + 4 wt% PVP | 2.0 ± 0.0 | -30.0 ± 1.7 | 1.8×10^{-3} | 1.9×10^{-6} |
| '' + 5 wt% PVP | 2.7 ± 0.0 | -31.5 ± 0.8 | 2.7×10^{-3} | 2.9×10^{-6} |
| '' + 2 wt% PVP (after 18 month) | 2.6 ± 0.3 | 27.1 ± 0.9 | 1.9×10^{-3} | 2.0×10^{-6} |
| '' + 3 wt% PVP (after 18 month) | 2.7 ± 0.1 | 24.0 ± 2.1 | 1.6×10^{-3} | 1.6×10^{-6} |
| '' + 4 wt% PVP (after 18 month) | 2.0 ± 0.1 | 23.1 ± 1.4 | 1.0×10^{-3} | 1.1×10^{-6} |
| '' + 5 wt% PVP (after 18 month) | 2.9 ± 0.2 | 22.4 ± 0.4 | 1.4×10^{-3} | 1.5×10^{-6} |

*) Figure of merit ZT was calculated for all composites with the thermal conductivity of PC/1 wt% MWCNT of $0.30 \text{ W/m}\cdot\text{K}$ [2]

Table S2. TE properties of PBT composites with SWCNT and PVP in different quantities (Volume conductivity, Seebeck coefficient, power factor, figure of merit ZT) measured at 40°C

| Composite | Vol. conductivity σ (S/m) | Seebeck coeff. S (μ V/K) | Power factor PF (μ W/(m·K ²)) | ZT* (-) |
|--------------------------------|-------------------------------------|----------------------------------|---|-------------------------------|
| PBT/ 2 wt% SWCNT [3] | 22.0 \pm 0.2 | 59.4 \pm 1.2 | 7.6 \times 10 ⁻² | 5.3 \times 10 ⁻⁵ |
| " + 2 wt% PVP | 14.7 \pm 7.6 | 25.0 \pm 0.5 | 9.2 \times 10 ⁻³ | 6.4 \times 10 ⁻⁶ |
| " + 4 wt% PVP | 8.2 \pm 0.1 | 18.4 \pm 0.7 | 2.8 \times 10 ⁻³ | 1.9 \times 10 ⁻⁶ |
| " + 6 wt% PVP | 9.0 \pm 5.0 | 11.2 \pm 1.2 | 1.1 \times 10 ⁻³ | 7.7 \times 10 ⁻⁷ |
| " + 8 wt% PVP | 8.3 \pm 3.3 | 7.9 \pm 0.8 | 5.2 \times 10 ⁻⁴ | 3.6 \times 10 ⁻⁷ |
| " + 10 wt% PVP | 4.0 \pm 0.0 | 18.3 \pm 1.5 | 1.3 \times 10 ⁻³ | 9.2 \times 10 ⁻⁷ |
| " + 2 wt% PVP (after 6 month) | 18.8 \pm 9.8 | 52.4 \pm 0.5 | 5.2 \times 10 ⁻² | 3.6 \times 10 ⁻⁵ |
| " + 4 wt% PVP (after 6 month) | 9.7 \pm 0.4 | 47.6 \pm 6.7 | 2.2 \times 10 ⁻² | 1.5 \times 10 ⁻⁵ |
| " + 6 wt% PVP (after 6 month) | 4.4 \pm 0.0 | 48.1 \pm 0.2 | 1.0 \times 10 ⁻² | 7.0 \times 10 ⁻⁶ |
| " + 8 wt% PVP (after 6 month) | 9.3 \pm 3.8 | 47.4 \pm 3.0 | 2.1 \times 10 ⁻² | 1.4 \times 10 ⁻⁵ |
| " + 10 wt% PVP (after 6 month) | 4.8 \pm 0.1 | 49.6 \pm 3.3 | 1.2 \times 10 ⁻² | 8.2 \times 10 ⁻⁶ |

*) Figure of merit ZT was calculated for all composites with the thermal conductivity of PBT/2 wt% SWCNT Tuball of 0.46 W/m·K

Table S3. TE properties of PEEK composites with SWCNT and PVP in different quantities (electrical volume conductivity, Seebeck coefficient, power factor, figure of merit ZT) measured at 40°C

| Composite | Vol. conductivity σ (S/m) | Seebeck coeff. S (μ V/K) | Power factor PF (μ W/(m·K ²)) | ZT* (-) |
|--------------------------------|-------------------------------------|----------------------------------|---|-------------------------------|
| PEEK/ 1 wt% SWCNT [1] | 6.2 | 48.0 \pm 1.3 | 1.4 \times 10 ⁻² | 1.1 \times 10 ⁻⁵ |
| " + 1 wt% PVP | 12.4 \pm 1.1 | 47.0 \pm 1.9 | 2.7 \times 10 ⁻² | 2.1 \times 10 ⁻⁵ |
| " + 2 wt% PVP | 12.9 \pm 0.8 | 49.7 \pm 6.2 | 3.2 \times 10 ⁻² | 2.5 \times 10 ⁻⁵ |
| " + 3 wt% PVP | 12.8 \pm 2.1 | 54.3 \pm 0.5 | 3.8 \times 10 ⁻² | 2.9 \times 10 ⁻⁵ |
| " + 1 wt% PVP (after 17 month) | 13.7 \pm 1.9 | 50.9 \pm 0.8 | 3.5 \times 10 ⁻² | 2.7 \times 10 ⁻⁵ |
| " + 2 wt% PVP (after 17 month) | 14.2 \pm 1.0 | 53.0 \pm 3.6 | 4.0 \times 10 ⁻² | 3.1 \times 10 ⁻⁵ |
| " + 3 wt% PVP (after 17 month) | 16.9 \pm 2.6 | 55.8 \pm 1.7 | 5.3 \times 10 ⁻² | 4.1 \times 10 ⁻⁵ |

*) Figure of merit ZT was calculated for all composites with the thermal conductivity of PEEK/1 wt% SWCNT Tuball of 0.40 W/m·K

Table S4. TE properties of PC composites with 2 wt% SWCNT and 15 wt% PVP (electrical volume conductivity, Seebeck coefficient, power factor, figure of merit ZT) measured at 40°C. Composite prepared by laboratory scale extrusion by project partner AIMEN (Spain)

| Composite | Vol. conductivity σ (S/m) | Seebeck coeff. S (μ V/K) | Power factor PF (μ W/(m·K ²)) | ZT* (-) |
|---------------------------------------|-------------------------------------|----------------------------------|---|-------------------------------|
| PC/2 wt% SWCNT+15 wt% PVP# | | | | |
| Direct after preparation (piece a) | 12.7 \pm 0.0 | 1.8 \pm 0.2 | 4.1 \times 10 ⁻⁵ | 4.3 \times 10 ⁻⁸ |
| after 3 month storage in air @25°C | 12.0 \pm 0.0 | 23.1 \pm 0.1 | 6.4 \times 10 ⁻³ | 6.7 \times 10 ⁻⁶ |
| Direct after preparation (piece b) | 26.0 \pm 0.1 | 0.7 \pm 0.1 | 1.1 \times 10 ⁻⁵ | 1.2 \times 10 ⁻⁸ |
| after 3 month storage in vacuum @25°C | 26.3 \pm 0.3 | 19.2 \pm 0.1 | 9.6 \times 10 ⁻³ | 1.0 \times 10 ⁻⁵ |

#) Preparation using Thermo Scientific HAAKE PolyLab QC lab conical twin-screw extruder with three heating zones (temperature profile: 190°C – 220°C – 230°C; dye temperature 220°C; rotation speed 10-20 rpm); premixing of components in a tubular: SWCNT and PVP for 15 min and then fillers with PC for 30 min

*) Figure of merit ZT was calculated for all composites with the thermal conductivity of PC/1 wt% MWCNT of about 0.3 W/m·K [2]

Determination of thermal conductivity:

The thermal conductivity of the composites was calculated from the product of thermal diffusivity, density, and specific heat capacity. The thermal diffusivity was measured on compression moulded round samples (diameter 12.3 mm, thickness 2 mm) through the plate thickness using the light flash apparatus LFA 447 NanoFlash (Netzsch-Gerätebau GmbH, Selb, Germany) at 25°C. The specific heat capacity of the composites was calculated by comparing the signal heights between the composite and the reference Pyroceram 9606 (with known specific heat capacity) using the LFA 447 NanoFlash. The density of composites was determined using a buoyancy method.

References

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