Supplemental Information on
Polymorphism of the Co-Te Nanophases in Mechanochemical Synthesis

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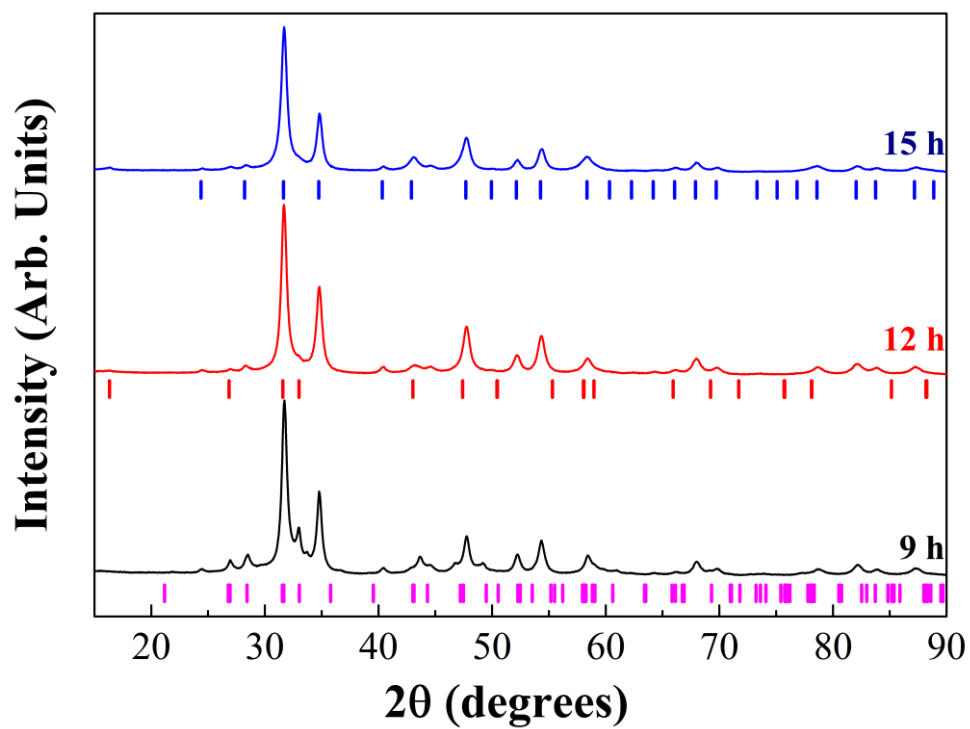
Figure S 1. Diffractograms obtained in the Bragg-Brentano reflection geometry, using a knife positioned above the sample to reduce the background. The time of milling is diplayed in the right side, the tick marker colors correspond to red CoTe$_2$ P-3m1, magenta to γ-CoTe2 Pnnm, blue to the α-CoTe$_2$ Pa-3.
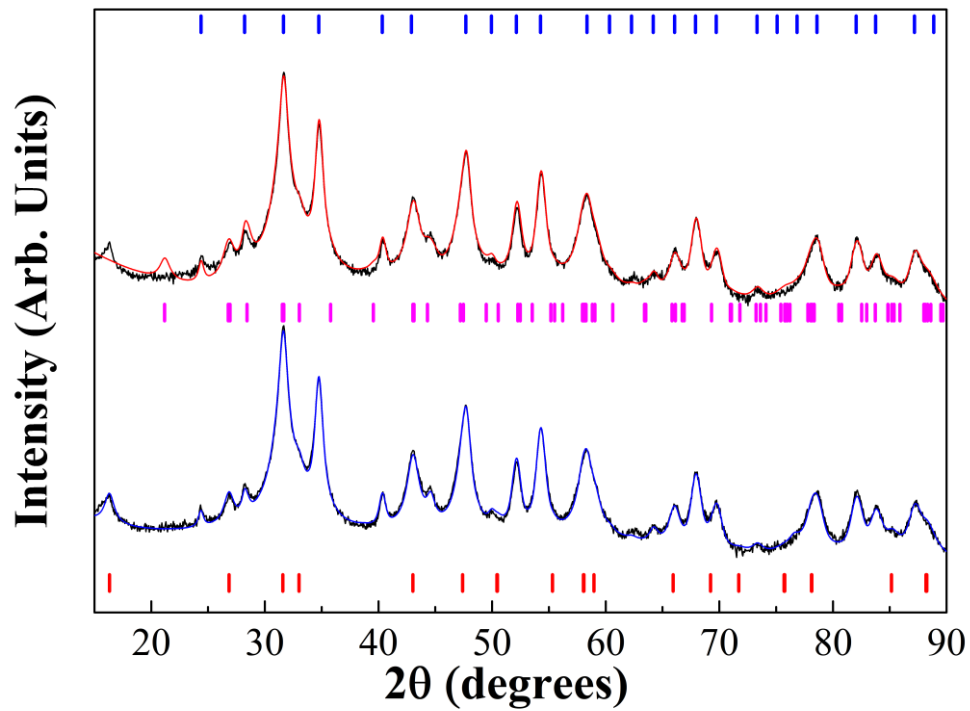
Figure S 2. Diffractogram of the $Co_{32}Te_{68}$ 15 h-milled sample with two different phase models: red curve uses the α-CoTe$_2$ Pa-3 (blue tick markers) and the γ-CoTe$_2$ Pnnm (magenta tick markers); the blue curve uses the CoTe$_2$ P-3m1 (red tick markers) instead of the latter. One can observe the misfit of the red curve signifying that the γ-CoTe$_2$ phase cannot be present in the material. The tick marker colors correspond to red CoTe$_2$ P-3m1, magenta to γ-CoTe2 Pnnm, blue to the α-CoTe$_2$ Pa-3.
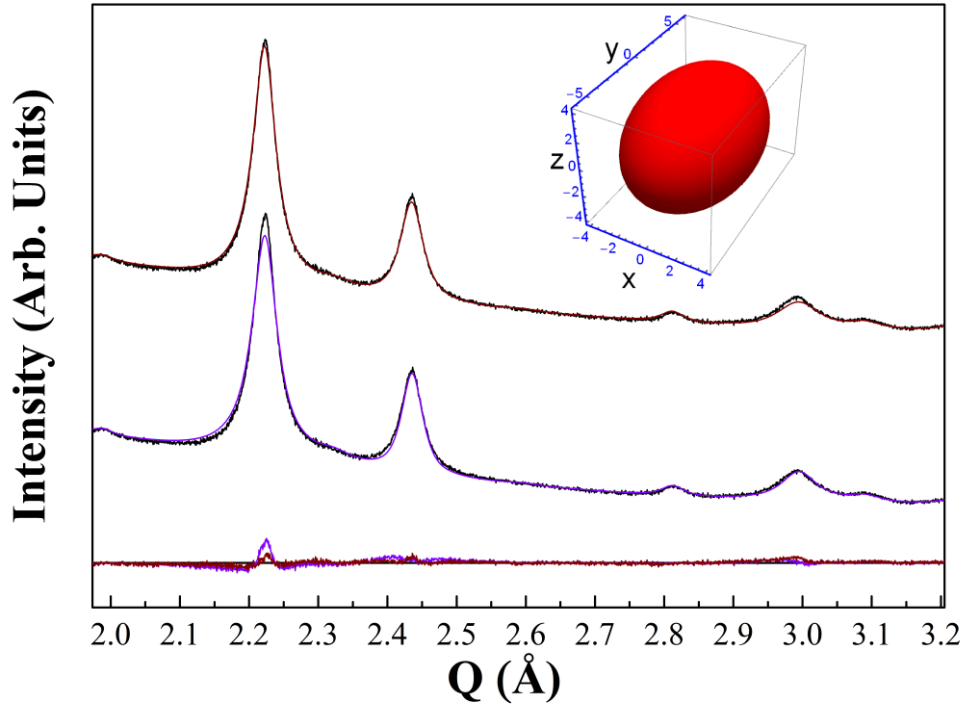
Figure S 3. Comparison of the DV and Anisotropic DV models for the LNLS data. The ellipsoid radii are $r_x=r_z=4.16(2)$ nm and $r_y= 6.11(7)$ nm, with x-direction parallel to [1 0 0].

Parameters	Spherical	$r_x=r_z{\neq}r_y$
$\mathcal{R}/\mathcal{R}_0$	1.088	1.0029
v_1	2	1
v_2	45	45
α (%)	2.24	66.8

Table S 1. Hamilton test applied for the ellipsoidal and spherical shapes.

$\mathcal{R}/\mathcal{R}_0$ represents the ratio between the more restricted model over the less restrictive one. $\mathcal{R}_0=R_{wp}=3.44$ when $r_x{\neq}r_y{\neq}r_z$.

v_1 means the difference between the number of parameters of the more restrictive model (spherical and $r_x=r_z$ constraint) over the less restrictive

v_2 represents the number of reflections minus the number of parameters refined of the less restrictive model.

α is the probability of the less restrictive model being wrong, which generally uses a cut-off of 5%, meaning that values above that signify the more restrictive model is right, which is observed for the $r_x=r_z$ case.
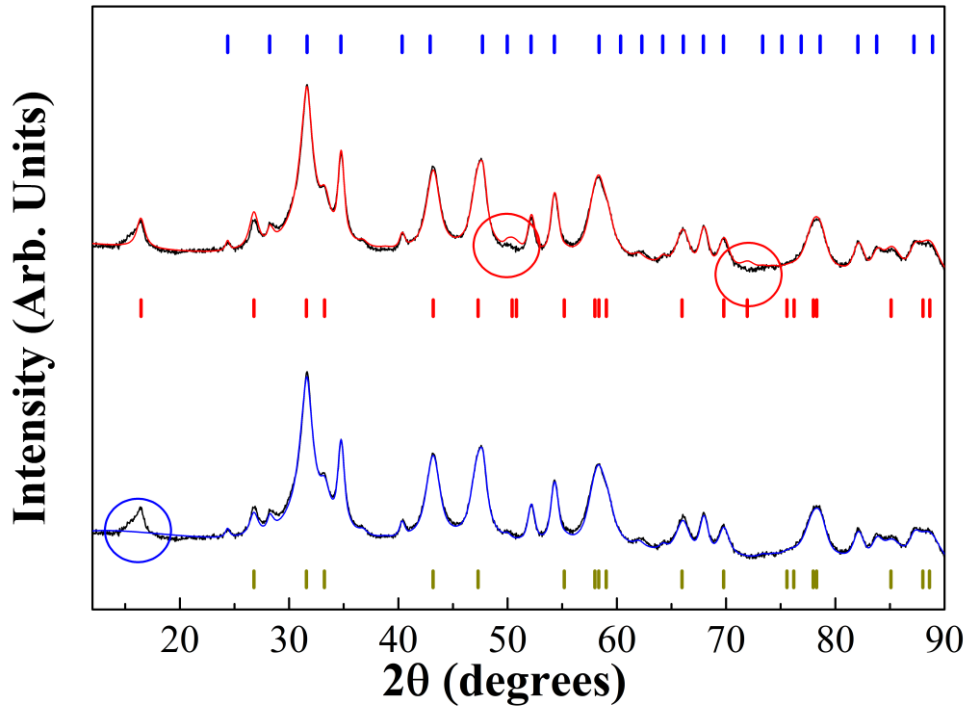

Figure S 4. Diffractograms of the $Co_{40}Te_{60}$ 15 h-milled sample with only two phases added. The red curve fits the $CoTe_2$ P-3m1 (red tick markers) and Pa-3 (blue tick markers) phases, showing some misfitting close to 2θ 50 and 70º (circled). The blue curve corresponds to the β-CoTe (yellow tick markers) and $CoTe_2$ Pa-3 model, which does not show unexpected peaks although cannot describe the peak near 2θ 15º (circled).
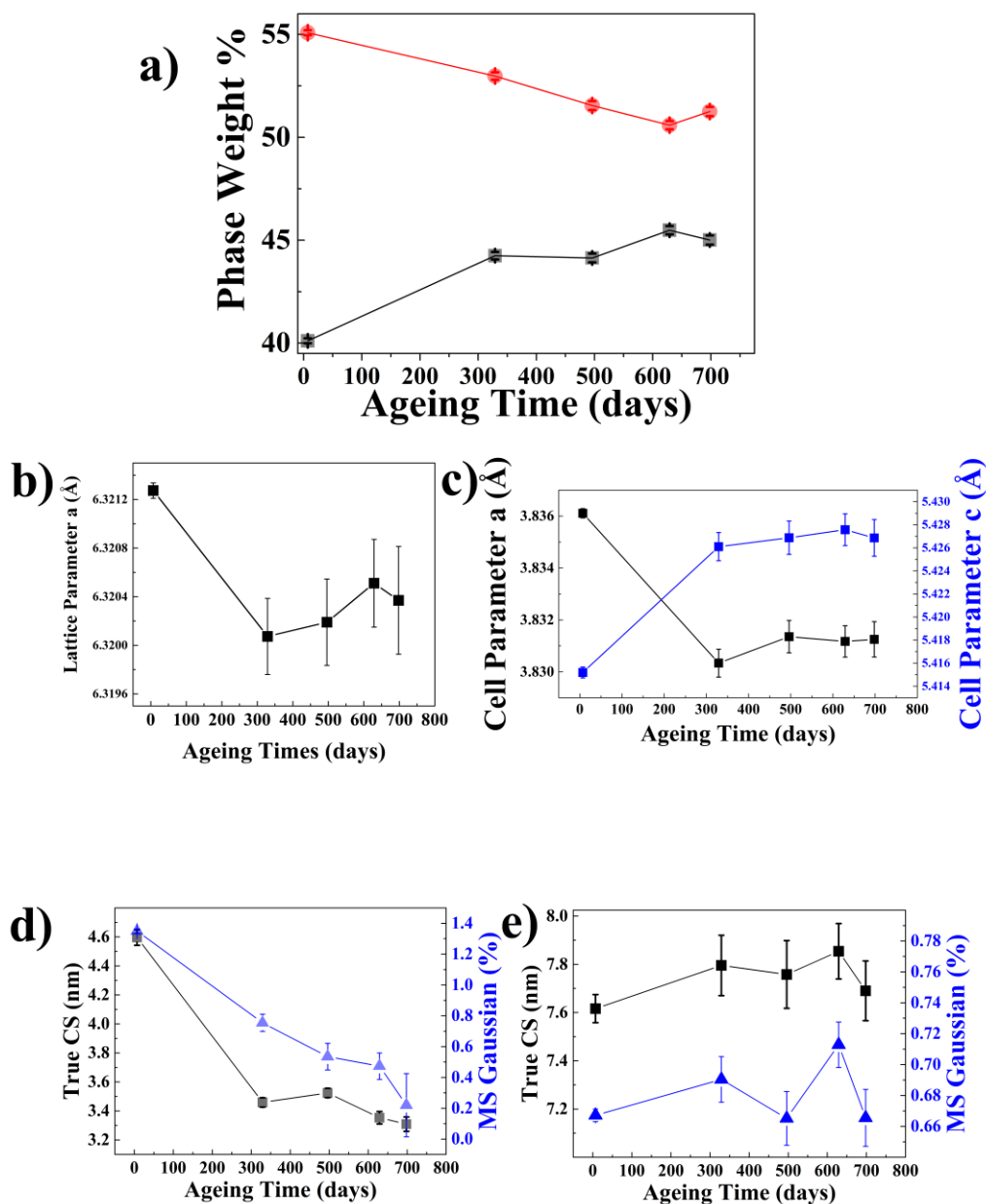
Figure S 5. Phase percentage, structural and microstructural information of the $Co_{32}Te_{68}$ 15 h-milled sample. The data used were collected using a knife to reduce the air scattering, apart from the first point, which used the synchrotron data. a) Phase weight percentage obtained with the anisotropic DV model. Red stands for $CoTe_2$ Pa-3 phase and black for $CoTe_2$ P-3m1. b) Lattice parameters of the $CoTe_2$ Pa-3 phase. c) Cell parameters of the $CoTe_2$ P-3m1 phase. d) Microstructural information of the P-3m1 structure. e) Microstructure of the Pa-3 phase.
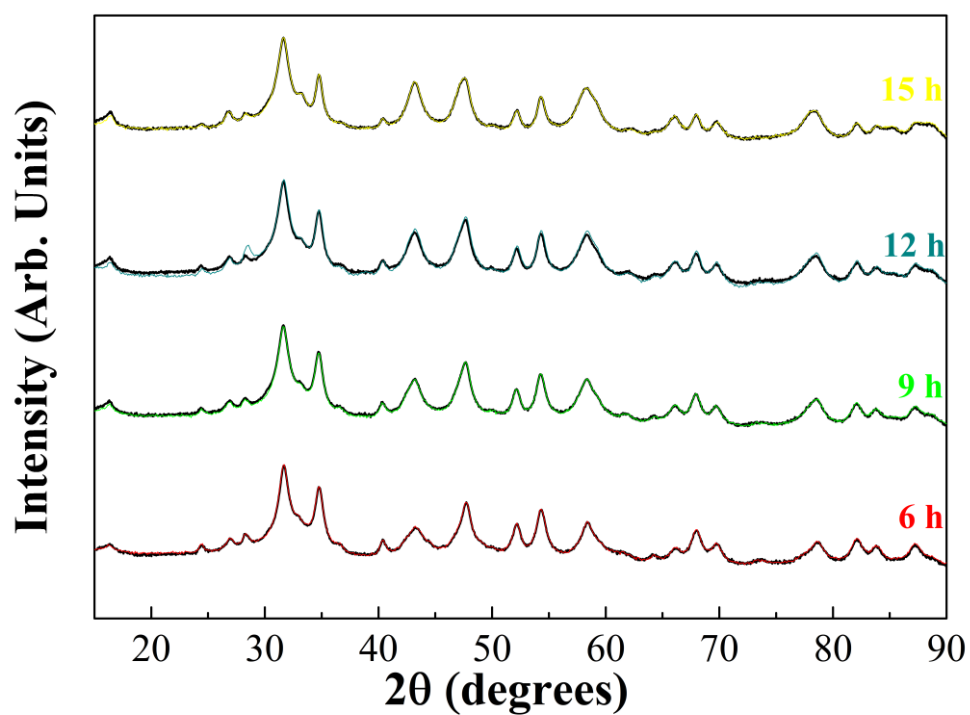
Figure S 6. Comparison of the diffractograms obtained after 10 months (black) of the synthesis and after 2 years (colored) for the $Co_{40}Te_{60}$ samples. The exception is the 12 h-milled sample which was measured 6 months after the synthesis, with 1° of fixed divergent slits, which is the main cause of the intensity differences. No phase transition is observed and no big differences in the structural (peak positions) and microstructure (peak widths) are distinguishable.