Structural, microstructural and magnetic characterization of β-CoTe nanophase synthesized by a novel mechanochemical method

Marcelo Augusto Malagutti¹, Kelli de Fátima Ulbrich¹, V. Z. C. Paes², J. Geshev², Carlos Eduardo Maduro de Campos ^{1,a}

¹ Departamento de Física, Universidade Federal de Santa Catarina, 88040-970 Florianópolis, Brazil

² Instituto de Física, Universidade Federal do Rio Grande do Sul, Porto Alegre 91501-970, Rio Grande do Sul, Brazil

E-mail: a carlos.campos@ufsc.br,



Figure S 1. XRPD patterns in logarithmic scale of CoTe milled for 15 hours and their Rietveld profile fitting. Red graph is the measurement with knife and black is the one without it. The colored curves on top of them represent their Rietveld fittings. In the bottom of the graph one can see the difference between calculated and measured diffractograms. Red numbers represent β -CoTe phase, black CoO, purple Co, and blue Fe.



Figure S 2. 12h-milled sample diffractogram. The colors represent the same parameters from the S 1 Figure.



Figure S 3. 9h-milled sample diffractogram. The colors represent the same parameters from the S 1 Figure.



Figure S 4. 6h-milled sample diffractogram. The colors represent the same parameters from the S 1 Figure.



Figure S 5. Zoom of the 15h-milled sample in the normal scale. Red stands for the measured data, blue (green) for the TOPAS profile fit with (out) Fe.



Figure S 6. Granular Te manually grinded diffractogram. The red ticks correspond to the Te P3121 phase and black to the α -TeO₂ (P41212). The Rwp reached 17.33, Rwp' 22.91, and GoF 3.70. The Tellurium Oxide represents 2% of the total mass phase percentage.



Figure S 7. a) XRPD patterns ageing time comparison with monochromator and a knife. Black represents 7 days after the milling, red 77 days and blue 200 days. The blue curve was multiplied by a 1.78 factor to compensate for the one scan short measurement. All the equipment settings were described in the article. b) Microstructure information, black square represents the CS and the triangles the MS. c) Lattice parameter a evolution with age and d) corresponds to the lattice parameter c ageing.



Figure S 8. Diffractograms obtained by XRPD of the second batch showing the samples' evolution with milling time. The tick markers represent the Bragg reflections, red stands for the β -CoTe, blue for Fe, magenta for Co, and black for CoO. No background subtraction was performed.



Figure S 9. Symbols: descending branches of the $M \times H$ loops obtained at different temperatures via PPMS measurements for the $Co_{50}Te_{50}$ sample ball-milled for 15h; the lines are the respective fitting curves.



Figure S 10 FC/ZFC curves in an applied field of 100 Oe of the Co50Te50 15h-milled sample.