

Supporting Information

for

Synthesis and characterization of quaternary La(Sr)S-TaS₂ misfit-layered nanotubes

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Beilstein J. Nanotechnol. 2019, 10, 1112-1124. doi:10.3762/bjnano.10.111

Additional experimental data and calculations

Table S1. Diameter distribution of the tubes

Sample	Average Inner Diameter (nm)	Average Outer diameter (nm)	Number of Tubes Analyzed
Sr_xLa_{1-x} - TaS_2	38	134	18
$\frac{(10 \text{ at\% Sr})}{\text{Sr}_{x}\text{La}_{1-x}\text{-TaS}_{2}}$	47	133	9
(20 at% Sr)	.,	133	
Sr_xLa_{1-x} - TaS_2	78	216	14
(40 at% Sr)			
Sr_xLa_{1-x} - TaS_2 (60 at% Sr)	64	195	12

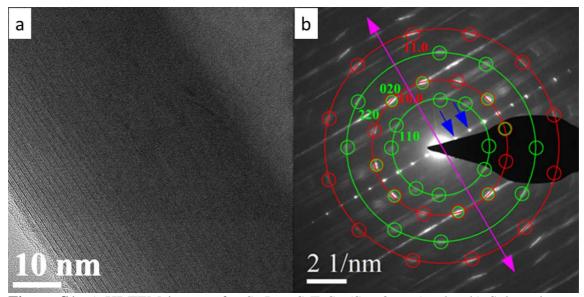


Figure S1. a) HRTEM image of a $Sr_xLa_{1-x}S$ -TaS₂ (Sr 60 at%) tube, b) Selected area diffraction showing the orientation relationship between $Sr_xLa_{1-x}S$ layers (green) and TaS₂ layers (red). The tube axis is shown as pink arrow and the basal reflections are marked with blue arrows.

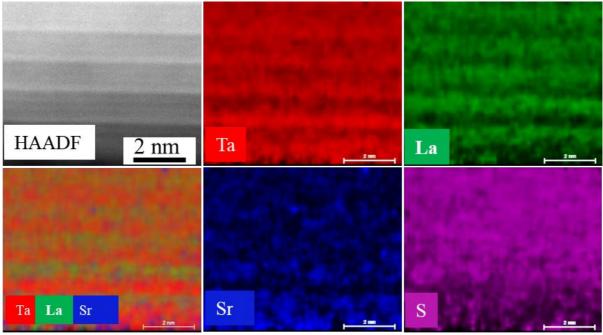


Figure S2. HAADF STEM image and EDX elemental mapping on a $Sr_xLa_{1-x}S$ - TaS_2 tube synthesized with Sr 60 at% in the precursor.

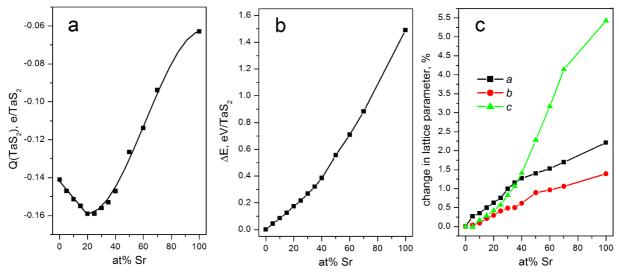


Figure S3. (a) The variations in the amount of charge transfer from $Sr_xLa_{1-x}S$ to TaS_2 within $Sr_xLa_{1-x}S$ - TaS_2 misfits (Q), (b) the relative formation energies (ΔE) and (c) the lattice parameters (a, b, c), depending on the Sr content. DFT calculations.

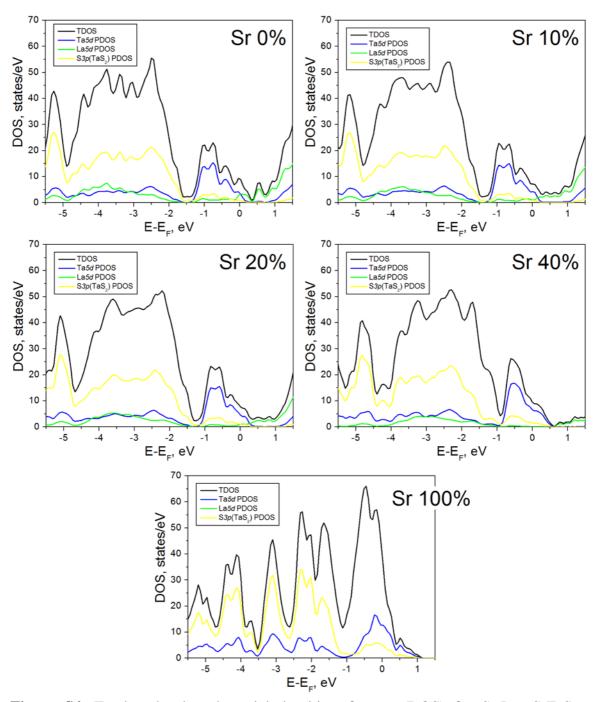


Figure S4. Total and selected partial densities-of-states (DOS) for $Sr_xLa_{1-x}S-TaS_2$ misfits with different Sr content. DFT calculations.