Supporting Information

Exploring the Structure and Properties of $V_wSe_yTe_{2-y}$ Mixed Crystals in the VTe_2–VSe_2 System

Sophia Kurig [1,†], Fabian Ketter [1,†], Anne Frommelius [1], B. Viliam Hakala [2], Jan van Leusen [1], Karen Friese [2] and Richard Dronskowski [1,3,*]

Table S1. Spatial parameters of $V_{1.13}Se_{0.72}Te_{1.28}$ and $V_{1.10}Se_{0.42}Te_{1.58}$. The refined Se occupancies are designated with $\varepsilon_1 = 0.36(3)$ and $\varepsilon_2 = 0.21(3)$.

Atom	Position	x	y	z	Occupancy	U_{eq} (Å²)
		$V_{1.13}Se_{0.72}Te_{1.28}$				
V1	1*a*	0	0	0	1	0.0582(13)
V2	1*b*	0	½	0	0.128(11)	0.028(6)
Se	2*d*	⅓	⅔	0.235(3)	ε_1	0.0212(7)
Te	2*d*	⅓	⅔	0.265(1)	$1 - \varepsilon_1$	"
		$V_{1.10}Se_{0.42}Te_{1.58}$				
V1	1*a*	0	0	0	1	0.0469(10)
V2	1*b*	0	½	0	0.099(12)	0.035(8)
Se	2*d*	⅓	⅔	0.214(3)	ε_2	0.0088(16)
Te	2*d*	⅓	⅔	0.266(1)	$1 - \varepsilon_2$	0.0186(5)

Differential scanning calorimetry (DSC) and thermogravimetric analysis (TGA) measurements

The investigation at elevated temperatures was performed using simultaneous thermal analysis (STA) which combines thermogravimetric analysis (TGA) and differential scanning calorimetry (DSC). The experiments were conducted on a STA PT1600 from LINSEIS Messgeräte GmbH (Selb, Germany). Measurements were performed in nitrogen 5.0 atmosphere and the samples placed into Al_2O_3 crucibles covered with a perforated lid.

Under these conditions, the $VSe_{0.72}Te_{1.28}$ showed an endothermic peak at a temperature of 850 °C in DSC while a mass loss in TGA was observed (Figure S1). At the same temperature after the main mass loss, a second event giving a slight increase in mass was observed, indicating the formation of a new phase formed with the surrounding gas. The powder XRD analysis of the thermally treated sample showed that the sample had decomposed partially and formed VN (Figure S2). With increasing temperature, an exothermic signal most likely due to thermal expansion of the powdery sample was observed. Possibly, this rearrangement results in a closer packing. While in literature it was reported that VN forms at 1100 °C here, we see a partial decomposition already at a 250 °C lower temperature [36,37].

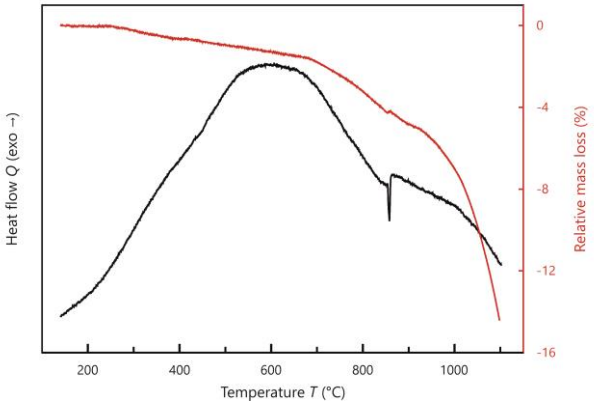

Figure S1. Thermogravimetric analysis and differential scanning calorimetry of $VSe_{0.72}Te_{1.28}$ with percentage of mass loss in red and heat flow in black.

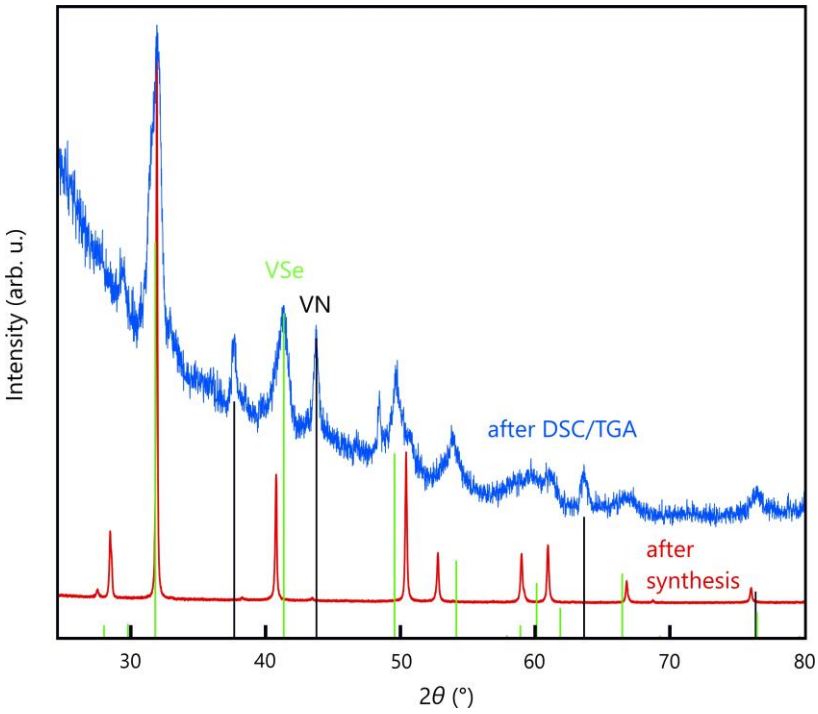

Figure S2. Comparison of $VSe_{0.72}Te_{1.28}$ powder X-ray data after synthesis (red), after DSC/TGA (blue), and Bragg positions of VSe [34] (green) and VN [35] (black).

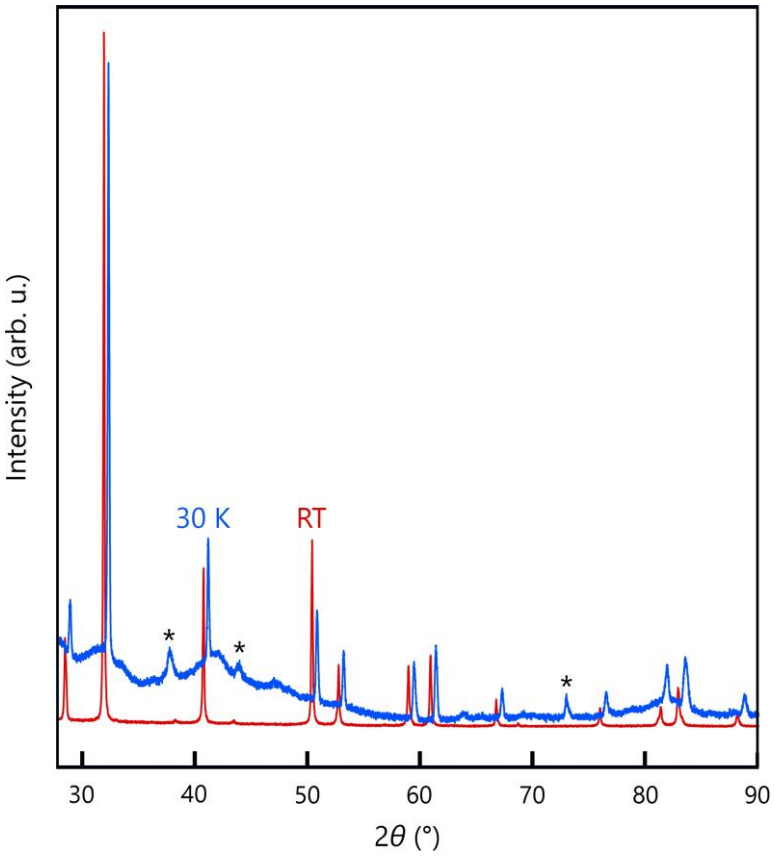

Figure S3. Comparison of $VSe_{0.72}Te_{1.28}$ powder X-ray data at room temperature in red and at 30 K in blue. The asterisks mark additional reflections, most likely of the sample holder.