MS23-P09 | INCOMMENSURATELY MODULATED STRUCTURES IN THE SERIES $RETe_{2-\delta}$

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Rare earth metal polychalcogenides $REX_{2-\delta}$ (X = S, Se, Te; $0 \leq \delta \leq 0.2$) comprise puckered [REX] double layers and planar [X] layers, the latter being subject to modulations due to electronic reasons and chalcogen defects [1].

The main reflections of all $RETe_{2-\delta}$ crystals correspond to an average ZrSSi type (space group $P4/nmm$) with unit cell with cell dimensions of $a \approx 440$ to 450 pm and $c \approx 910$ to 920 pm. Satellite positions, however, vary with δ. The structures of $RETe_{1.9}$ (RE = La, Pr, Nd) compounds can be described in the tetragonal superspace group $P4/n(\alpha\beta1/2)00(-\beta\alpha1/2)00$ with modulation vectors $q_1 \approx (0.26,0.32,1/2)$ and $q_2 \approx (-0.32,0.26,1/2)$, whereas $LaTe_{1.8}$ is orthorhombic, superspace group $Pmmn(\alpha\beta1/2)000$ $(-\alpha\beta1/2)000$ as its modulation vectors $q_1 = (0.275,0.31,1/2)$ and $q_2 = (-0.275,0.31,1/2)$ are incompatible with fourfold rotational symmetry.

The Te layers of the $RETe_{1.9}$ compounds show a displacive and occupational modulation, forming an array of vacancies, Te_2^{2-} anions and linaer Te_3^{4-} anions. For $LaTe_{1.8}$, the modulation in the Te layers is more pronounced with a variety of different Te anions.

[1] T. Doert, C. J. Müller: Binary Polysulfides and Polyselenides of Trivalent Rare-Earth Metals, in: *Reference Module in Chemistry, Molecular Sciences and Chemical Engineering*, Elsevier, **2016**.