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# Crystal structure of the $RAgTe_2$ (R = Y, Tb, Dy, Ho and Er) compounds

L.D. Gulay [a,*], I.D. Olekseyuk [a], A. Pietraszko [b]

[a] *Department of General and Inorganic Chemistry, Volyn State University, Voli Avenue 13, 43009 Lutsk, Ukraine*

[b] *W. Trzebiatowski Institute of Low Temperature and Structure Research, Polish Academy of Sciences, Okólna Street 2, P.O. Box 1410, 50-950 Wrocław, Poland*

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**Abstract**

The crystal structures of the $RAgTe_2$ (R = Y, Tb, Dy, Ho and Er) compounds (space group $P\bar{4}2_1m$, Pearson symbol *tP8*) were determined by means of X-ray powder diffraction: $a = 0.71398(2)$ nm, $c = 0.45947(2)$ nm, $R_I = 0.0701$ ($YAgTe_2$), $a = 0.71466(3)$ nm, $c = 0.46108(3)$ nm, $R_I = 0.0761$ ($TbAgTe_2$), $a = 0.71287(3)$ nm, $c = 0.45955(3)$ nm, $R_I = 0.0637$ ($DyAgTe_2$), $a = 0.71033(3)$ nm, $c = 0.45713(3)$ nm, $R_I = 0.0755$ ($HoAgTe_2$) and X-ray single crystal diffraction: $a = 0.7091(1)$ nm, $c = 0.45650(9)$ nm, $R_1 = 0.0366$ ($ErAgTe_2$). The Te atoms in the structure of the $RAgTe_2$ compounds are stacked in a close-packed arrangement with layers in the sequence AB. Half of the octahedral interstices are occupied by the R atoms. The Ag atoms are located in remaining octahedral interstices, but they are shifted from the centers of the respective octahedra and tetrahedral surrounding really exists for Ag.


*Keywords:* Chalcogenides; Rare earth compounds; Ag compounds; Te compounds; Crystal structure; X-ray single crystal diffraction; X-ray powder diffraction

## 1. Introduction

The rare-earth chalcogenides are being intensively studied due to their specific thermal, electrical and optical properties, which e.g. make them prospective materials in the field of infrared and nonlinear optics. Investigation of the crystal structures of complex chalcogenides is important step of a searching of new materials with interesting properties.

The formation of ternary $RAgTe_2$ (R = Y, Gd, Dy, Ho, Er and Tm) compounds has been reported in Refs. [1,2]. Tetragonal symmetry and lattice parameters have been reported. No crystal structure determination for these compounds has been reported in literature.

In the course of our systematic investigation on rare-earth tellurides with transition metals we reported recently on the formation of new compounds $R_7Cu_3Te_{12}$ (R = Y, Tb, Dy, Ho, Er and Tm) ($Ho_7Cu_3Te_{12}$ structure type, space group $R\bar{3}m$) [3,4] and $RCu_3Te_3$ (R = Er and Tm) ($RCu_3Te_3$ structure type, space group $Pmn2_1$) [5].

In present paper the crystal structures of ternary $RAgTe_2$ (R = Y, Tb, Dy, Ho and Er) compounds of tetragonal symmetry are reported and discussed at the first time.

## 2. Experimental details

The samples were prepared using high purity elements (the purity of the ingredients was better than 99.9 wt.%). The calculated amounts of the components were sealed in evacuated silica ampoules. The synthesis was realized in a tube furnace. The ampoules were heated with the heating rate of 30 K/h to maximal temperature 1420 K. The samples were kept at maximal temperature during 4 h. After that they were cooled slowly (10 K/h) to 870 K and annealed at this temperature during 240 h. After annealing the ampoules with the samples were quenched in air.

Diffraction-quality single crystal of the $ErAgTe_2$ compound for the crystal structure determination was selected from the sample of the respective composition. The X-ray diffraction data were obtained with the use of graphite-monochromatized Mo Kα radiation ($\lambda = 0.071073$ nm) on a KUMA diffraction KM-4 four-circle single crystal diffractometer equipped with CCD camera. The intensities of the reflections were corrected for Lorentz and polarisation factors. Semiempirical absorption correction was applied. The crystal structure was solved by Patterson methods [6] and refined by full matrix least squares method using SHELX-97 program [7].

X-ray powder diffraction patterns of the $RAgTe_2$ (R = Y, Tb, Dy, Ho and Er) compounds were recorded using automatic powder diffractometer DRON-4-13 (Cu Kα radiation, $10^\circ \leq 2\Theta \leq 100^\circ$, step scan mode with a step size of 0.05° and counting time of 20 s per data point). Crystal structure determination was performed using the CSD [8] program.

## 3. Results and discussion

The formation of the $RAgTe_2$ (R = Y, Tb, Dy, Ho and Er) compounds was observed during the investigation of the phase

* Corresponding author.
*E-mail address:* gulay@univer.lutsk.ua (L.D. Gulay).

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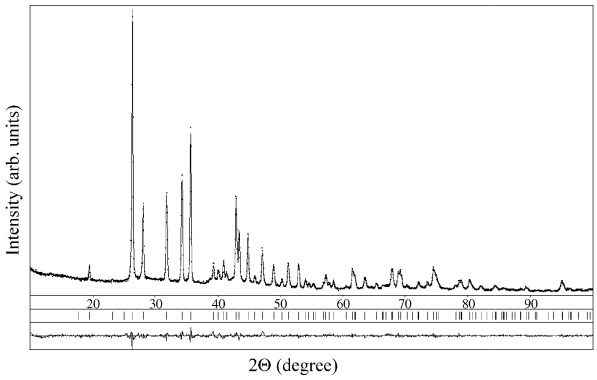


Fig. 1. The experimental and calculated diffractograms and the corresponding difference diagram for $YAgTe_2$.

relations in the respective $R_2Te_3$–$Ag_2Te$ systems. Single-phase samples of these compounds were obtained. Their X-ray powder diffraction patterns were similar. The crystal structure of the $ErAgTe_2$ compound was investigated using X-ray single crystal diffraction. The extinctions observed were found to be consistent with the space group $P\bar{4}2_1m$ which was applied for the crystal structure solution and refinement. The crystal data and refinement information on the $ErAgTe_2$ compound are summarized in Table 1, whereas positional and thermal parameters are given in Table 2. One position of Er, one position of Ag and one

Table 1
Crystal data and structure refinement details of the $ErAgTe_2$ compound

| | |
|---|---|
| Empirical formula | $ErAgTe_2$ |
| Formula weight | 530.33 |
| Space group | $P\bar{4}2_1m$ (No. 113) |
| Unit cell dimensions (nm) | $a = 0.7091(1)$, $c = 0.45650(9)$ |
| Volume ($nm^3$) | 0.22954(6) |
| Number of formula units per unit cell | 2 |
| Calculated density ($g/cm^3$) | 7.673 |
| Absorption coefficient ($mm^{-1}$) | 34.661 |
| $F(0\,0\,0)$ | 438 |
| Crystal size (mm) | $0.08 \times 0.09 \times 0.12$ |
| $\Theta$ range for data collection | 4.06–25.67 |
| Index ranges | $-8 \le h \le 7$, $-8 \le k \le 8$, $-5 \le l \le 5$ |
| Reflections collected | 2412 |
| Independent reflections | 252 [$R$(int.) = 0.0808] |
| Refinement method | Full-matrix least-square on $F^2$ |
| Absolute structure parameter | 0.00(6) |
| Data/restraints/parameters | 252/0/15 |
| Goodness-of-fit on $F^2$ | 1.041 |
| Final $R$ indices [$I > 2\sigma(I)$] | $R_1 = 0.0366$, $wR_2 = 0.1075$ |
| $R$ indices (all data) | $R_1 = 0.0378$, $wR_2 = 0.1094$ |
| Extinction coefficient | 0.002(1) |
| Largest diff. peak and hole $\times 10^{-3}$ ($e/nm^3$) | 2.729 and −1.800 |

Table 2
Atomic coordinates and temperature factors for the $ErAgTe_2$ compound

| Atom | Position | $x/a$ | $y/b$ | $z/c$ | $U_{eq.} \times 10^2$ ($nm^2$) | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{23}$ | $U_{13}$ | $U_{12}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| Er | 2(c) | 0 | 1/2 | 0.7971(3) | 0.0191(6) | 0.0205(6) | 0.0205(6) | 0.0165(9) | 0 | 0 | 0.0006(5) |
| Ag | 2(a) | 0 | 0 | 0 | 0.0352(8) | 0.036(1) | 0.036(1) | 0.033(1) | 0 | 0 | 0 |
| Te | 4(e) | 0.7972(1) | 0.2972(1) | 0.2873(4) | 0.0204(6) | 0.0215(6) | 0.0215(6) | 0.0183(9) | −0.0006(4) | −0.0006(4) | −0.0038(6) |

$U_{eq.}$ is defined as one third of the trace of the orthogonalized $U_{ij}$ tensor. The anisotropic temperature factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11} + \cdots + 2hka^*b^*U_{12}]$.

Table 3
Crystal data and structure refinement details of the $RAgTe_2$ (R = Y, Tb, Dy and Ho) compounds

| Empirical formula | $YAgTe_2$ | $TbAgTe_2$ | $DyAgTe_2$ | $HoAgTe_2$ |
|---|---|---|---|---|
| Formula weight | 451.97 | 521.99 | 525.57 | 528.00 |
| Space group | $P\bar{4}2_1m$ (No. 113) | $P\bar{4}2_1m$ (No. 113) | $P\bar{4}2_1m$ (No. 113) | $P\bar{4}2_1m$ (No. 113) |
| Unit cell dimensions (nm) | $a = 0.71398(2)$, $c = 0.45947(2)$ | $a = 0.71466(3)$, $c = 0.46108(3)$ | $a = 0.71287(3)$, $c = 0.45955(3)$ | $a = 0.71033(3)$, $c = 0.45713(3)$ |
| Volume ($nm^3$) | 0.23423(2) | 0.23549(4) | 0.23353(3) | 0.23066(3) |
| Number of formula units per unit cell | 2 | 2 | 2 | 2 |
| Calculated density ($g/cm^3$) | 6.4080 | 7.361 | 7.473 | 7.602 |
| Absorption coefficient ($mm^{-1}$) | 152.263 | 202.774 | 208.329 | 167.862 |
| $F(0\,0\,0)$ | 380 | 432 | 434 | 436 |
| Diffractometer | Powder DRON-4-13 | Powder DRON-4-13 | Powder DRON-4-13 | Powder DRON-4-13 |
| $2\Theta$ range for data collection | 10.00–100.00 | 10.00–100.00 | 10.00–100.00 | 10.00–100.00 |
| Refinement method | Full profile | Full profile | Full profile | Full profile |
| $R_I$ | 0.0701 | 0.0761 | 0.0637 | 0.0755 |
| $R_P$ | 0.1048 | 0.1405 | 0.1398 | 0.1583 |
| Preferred orientation | [1 1 0] | [1 1 0] | [1 1 0] | [1 1 0] |
| Preferred orientation parameter | 0.76(1) | 0.79(4) | 1.03(5) | 1.10(1) |