Crystal structure of DyAg₃In₃

Marta DEMCHYNA¹*, Bohdana BELAN¹, Mykola MANYAKO¹, Lev AKSEL Rud¹, Antonio CERVELLINO², Viktor HLUKHYY³, Yaroslav KALYCHAK¹

¹ Faculty of Chemistry, Ivan Franko National University of Lviv, Kryyka i Mefodiya St. 6, UA-79005 Lviv, Ukraine
² Swiss Light Source, Paul Scherrer Institute, CH-5232 Villigen, Switzerland
³ Department of Inorganic Chemistry, Technical University of Munich, Lichtenberg St. 4, D-85747 Garching, Germany
* Corresponding author: E-mail: marta.dem.85@gmail.com

Received September 22, 2010; accepted October 29, 2010; available on-line March 2, 2011

The DyAg₃In₃ compound was prepared by arc-melting of pure compact metals under an argon atmosphere. The crystal structure was refined from synchrotron powder diffraction data (space group Im-3, a = 15.1472(2) Å, Z = 24, R_p = 0.0792, R_root = 0.1031, R_exp = 0.0231, refined composition DyAg₃In₃) and from conventional X-ray single crystal diffraction data (a = 15.1010(1) Å, R = 0.0423, R_root = 0.0433, refined composition DyAg₃83In₆7). The crystal structure belongs to the YbAg₃In₄ structure type, which is closely related to the structures of YbCd₆ and YCd₆.

Dysprosium/ Silver / Indium / Crystal structure / X-ray single crystal diffraction / Synchrotron X-ray diffraction

1. Introduction

Ternary compounds of rare-earth metals (RE) with 3d-metals and indium have recently attracted the attention of researchers, due to their interesting physical, mainly magnetic and electrical, properties [1]. The corresponding systems with 4d-, 5d- and noble metals are less studied, but several papers dedicated to them and their compounds have appeared in the last years [2-11].

In an earlier examination of the Yb–Ag–In system, the existence of the YbAg₃In₄ compound, which crystallizes in its own structure type, was discovered and its crystal structure and physical properties were investigated [12]. The compound has a relatively complex structure with a large lattice constant (a = 15.324 Å). The structure is defective with silver atoms occupying split-positions and is closely related to the binary intermetallics YCd₆ [13] and YbCd₆ [14]. A comparative analysis of the crystal structures of these compounds can be found in [12]. New representatives of the structure type are described in [15-18]. Phases with local pseudoicosahedral structure were found at the composition RE₆Ag₃In₄ (RE = Gd, Tb, Dy, Ho, Er, Tm, Yb and Lu) in [17]. Thermal and electrical properties of quasicrystals of the Yb–Ag–In system were studied in [18]. An X-ray single crystal investigation of the TbAg₃In₄ compound, isostructural with YbAg₃In₄, was performed in [19]. Formation of similar compounds has been revealed in several RE–Ag–In systems (RE = Ce, Pr, Eu, Gd, Tb, Dy, Er, Tm) [20] and an X-ray diffraction analysis of complex metallic alloys has been carried out for the Eu–Ag–In system [21]. Recently, a new series of REPd₃In₆ compounds (RE = Sm, Gd-Ho) with YbAg₃In₄ structure type was found [22].

During an investigation of the phase equilibria in the Dy–Ag–In system at 870 K the existence of a ternary compound of composition DyAg₃In₃ was confirmed. The determination of the crystal structure of this compound by means of conventional X-ray single crystal diffraction and synchrotron powder diffraction is the object of this work.

2. Experimental

Samples for the investigation were prepared by arc melting under an argon atmosphere (purified with a titanium getter) from compact metals of high purity: Dy 99.8 wt.%, Ag 99.98 wt.%, and In 99.999 wt.%. Homogeneous annealing was performed at 870 K for one month. High-resolution powder diffraction data were collected for an annealed alloy of composition Dy₁₅Ag₃In₁₂ at room temperature (0.5 mm glass capillary). Synchrotron radiation (Materials Science Beamline at the SLS, PSI: silicon strip detector
Table 1 Experimental and crystallographic data for DyAg\textsubscript{3}In\textsubscript{3}.

<table>
<thead>
<tr>
<th>Composition</th>
<th>DyAg\textsubscript{3}In\textsubscript{3}</th>
<th>YbAg\textsubscript{3}In\textsubscript{3}</th>
<th>DyAg\textsubscript{3}In\textsubscript{3}</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mr, g mol\textsuperscript{-1}</td>
<td>831.634</td>
<td>814.701</td>
<td>814.701</td>
</tr>
<tr>
<td>Structure type</td>
<td>YbAg\textsubscript{3}In\textsubscript{3}</td>
<td>YbAg\textsubscript{3}In\textsubscript{3}</td>
<td>YbAg\textsubscript{3}In\textsubscript{3}</td>
</tr>
<tr>
<td>Space group</td>
<td>Im-3 (204)</td>
<td>Im-3 (204)</td>
<td>Im-3 (204)</td>
</tr>
<tr>
<td>Z; Pearson code</td>
<td>24; c \text{168}.240 \text{ Å} \text{c}</td>
<td>24; c \text{164}.472 \text{ Å} \text{c}</td>
<td>24; c \text{164}.472 \text{ Å} \text{c}</td>
</tr>
<tr>
<td>Lattice parameter, Å</td>
<td>a = 15.1472(2) \text{ Å}</td>
<td>a = 15.1010(1) \text{ Å}</td>
<td>a = 15.1010(1) \text{ Å}</td>
</tr>
<tr>
<td>Cell volume, Å\textsuperscript{3}</td>
<td>3475.3(2) \text{ Å} \text{c}</td>
<td>3443.64(7) \text{ Å} \text{c}</td>
<td>3443.64(7) \text{ Å} \text{c}</td>
</tr>
<tr>
<td>Crystal size, µm</td>
<td>–</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td>Color</td>
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<td>metallic dark gray</td>
<td>metallic dark gray</td>
</tr>
<tr>
<td>Calculated density, g cm\textsuperscript{-3}</td>
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<td>9.4238(2)</td>
<td>9.4238(2)</td>
</tr>
<tr>
<td>Radiation type; wavelength, Å</td>
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<td>Mo K\textalpha; 0.71073</td>
<td>Mo K\textalpha; 0.71073</td>
</tr>
<tr>
<td>Absorption coefficient, mm\textsuperscript{-1}</td>
<td>383.49</td>
<td>341.33</td>
<td>341.33</td>
</tr>
<tr>
<td>Range in hkl</td>
<td>–</td>
<td>1159/791</td>
<td>1159/791</td>
</tr>
<tr>
<td>Reflections collected/unique</td>
<td>2θ\text{min}-2θ\text{max}, deg.</td>
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<td>2.59-76.89</td>
</tr>
<tr>
<td>Refinement method</td>
<td>full profile</td>
<td>full-matrix least-squares</td>
<td>full-matrix least-squares</td>
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<tr>
<td>Refined parameters</td>
<td>65</td>
<td>44</td>
<td>44</td>
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<tr>
<td>Goodness-of-fit on F\textsuperscript{2}</td>
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<td>1.06</td>
<td>1.06</td>
</tr>
<tr>
<td>Final R indices [\textgreater 2\textsigma(I)]</td>
<td>Rp = 0.0792, Rp = 0.1031</td>
<td>Rp = 0.0423, Rwp = 0.0433</td>
<td>Rp = 0.0423, Rwp = 0.0433</td>
</tr>
</tbody>
</table>

\*Impurities: 2 – DyIn\textsubscript{3} phase (18.92 wt.% AuCu\textsubscript{7}-type, space group \textit{Pm}-3\textit{m}, a = 4.5364(2) Å), 3 – Ag-In\textsubscript{3} phase (2.73 wt.% Mg-type, space group \textit{P6}3\textit{mmc}, a = 3.0044(4), c = 4.7668(4) Å).

MYTHEN II) with a wavelength of \( \lambda = 0.49063 \) Å was used. The diffractometer was calibrated with an external silicon standard.

A single crystal of irregular shape was selected mechanically from the same alloy. Single crystal diffraction data were collected on an Xcalibur 3 diffractometer (Oxford Diffraction) equipped with a monochromatic Mo K\textalpha\ source (\( \lambda = 0.71073 \) Å). The exposure time was 80 s per frame. The collection of intensity data was carried out with the CrysAlis program. The final lattice parameters were calculated from all the observed reflections in the actual data collection. The structure was solved by direct methods, and refined by using the WinCSD program package [23]. The crystallographic data and details of the data collection are listed in Table 1.

The single crystal investigated on the diffractometer was also studied by energy-dispersive X-ray analysis (EDX), using a Leica420i scanning electron microscope.

3. Results and discussion

Based on the results of the phase analysis of the alloys of Dy–Ag–In system, the composition of the investigated compound was found to be REAg\textsubscript{3}In\textsubscript{3}, as for the TbAg\textsubscript{3}In\textsubscript{3} compound [19]. The composition was confirmed by EDX analysis of the surface of the single crystal. Experimental data and the results of the X-ray synchrotron powder diffraction analysis (Fig. 1) and the X-ray (Mo K\textalpha\) single crystal diffraction analysis are shown in Table 1. It should be noted that the powder specimen contained small amounts of DyIn\textsubscript{3} (18.92 wt.%) [24] and Ag-In\textsubscript{3} (2.73 wt.%) [25] (Fig. 1). The refined unit cell parameters determined from the synchrotron powder diffraction data (15.1472(2) Å) agree well with the values reported in [17] (15.17 Å) for an alloy of composition Dy\textsubscript{16}Ag\textsubscript{42}In\textsubscript{42} (conventional X-ray powder diffraction data), but are slightly higher than those obtained from the single crystal data (15.1010(1) Å). This indicates the possible existence of a small homogeneity range. Testing of various models based on both single crystal and powder diffraction data allowed us to assign the YbAg\textsubscript{3}In\textsubscript{3} structure type (space group \textit{Im}-3) to the DyAg\textsubscript{3}In\textsubscript{3} compound. The basic structure motif of these compounds is the same. However, part of the Wyckoff positions from single crystal data) and Tb-compounds. The site
Table 2 Atomic coordinates and isotropic displacement parameters for DyAg$_{3.010}$In$_3$ (synchrotron X-ray powder data – 1st row), DyAg$_{2.853}$In$_3$ (conventional X-ray single crystal data – 2nd row) and TbAg$_3$In$_3$ (conventional X-ray single crystal data [19] – 3rd row). Space group Im-3.

<table>
<thead>
<tr>
<th>Atom</th>
<th>Wyckoff position</th>
<th>Occ.</th>
<th>x</th>
<th>y</th>
<th>z</th>
<th>$B_{iso}$, Å$^2$</th>
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<tbody>
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<td>$^{1}$Dy</td>
<td>24g</td>
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<td>0</td>
<td>0.1868(2)</td>
<td>0.3032(2)</td>
<td>0.39(9)</td>
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<tr>
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<td>0</td>
<td>0.18611(9)</td>
<td>0.3030(1)</td>
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<td>0.31391(3)</td>
<td>–</td>
</tr>
<tr>
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<td>1</td>
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<td>0.1605(2)</td>
<td>0.1605(2)</td>
<td>2.32(9)</td>
</tr>
<tr>
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<td>0.1624(2)</td>
<td>0.1624(2)</td>
<td>0.1624(2)</td>
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<td>$^{3}$Ag1</td>
<td>16f</td>
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<td>0.1652(3)</td>
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<tr>
<td>$^{3}$Ag2</td>
<td>16f</td>
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<td>0.1515(6)</td>
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<tr>
<td>$^{1}$In1</td>
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<td>0.3477(3)</td>
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<td>0.3462(2)</td>
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<td>0.3462(2)</td>
<td>1.40(5)</td>
</tr>
<tr>
<td>$^{1}$In2</td>
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<td>0.76(2)</td>
<td>0</td>
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<td>0.0906(3)</td>
<td>1.2(2)</td>
</tr>
<tr>
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<td>0.13(2)</td>
<td>0</td>
<td>0.286(2)</td>
<td>0.083(2)</td>
<td>1.6(14)</td>
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<tr>
<td>$^{2}$Ag3</td>
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<td>0.0938(3)</td>
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<tr>
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<td>0.0954(7)</td>
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<tr>
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<td>0.2273(6)</td>
<td>0.0875(1)</td>
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</tr>
<tr>
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<td>0.0808(15)</td>
<td>0.0569(12)</td>
<td>0.1092(11)</td>
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</tr>
<tr>
<td>$^{2}$Ag5'</td>
<td>48h</td>
<td>0.086(1)</td>
<td>0.0904(11)</td>
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<td>0.0722(11)</td>
<td>0.75(11)</td>
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<tr>
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<td>0.053(3)</td>
<td>0.091(2)</td>
<td>0.055(3)</td>
<td>0.054(2)</td>
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<tr>
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<td>0.0892(5)</td>
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</tr>
<tr>
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<td>½</td>
<td>–</td>
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<tr>
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</tr>
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<td>$^{2}$Ag7</td>
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<td>0</td>
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<td>0.40988(8)</td>
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<tr>
<td>$^{1}$Ag8</td>
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<td>0</td>
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<td>0.2007(12)</td>
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</tr>
<tr>
<td>$^{2}$Ag8</td>
<td>12d</td>
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<td>–</td>
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</tr>
<tr>
<td>$^{1}$In1</td>
<td>24g</td>
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<td>0.3998(3)</td>
<td>0.3477(3)</td>
<td>1.6(2)</td>
</tr>
<tr>
<td>$^{2}$In1</td>
<td>24g</td>
<td>1</td>
<td>0</td>
<td>0.4025(2)</td>
<td>0.3462(2)</td>
<td>1.40(5)</td>
</tr>
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<td>$^{3}$In1</td>
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<td>1</td>
<td>0</td>
<td>0.40263(5)</td>
<td>0.3462(2)</td>
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</tr>
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<td>0.20274(4)</td>
<td>0.11760(4)</td>
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</tr>
</tbody>
</table>

splitting is typical for the Ag3,4 atoms for both compounds, however for the Tb compound the total occupancy was equal to 1, whereas for the Dy compound it is slightly lower (0.89 for the powder diffraction data and 0.96 for the single crystal data). Only the refinement on single crystal diffraction data show site splitting for the Ag5 (Ag5') atoms for the DyAg$_3$In$_3$ compound, but the site occupancy 0.14 agrees well with the results obtained by X-ray powder diffraction and with the results for TbAg$_3$In$_3$. Another difference is observed for the 16f position occupied by Ag1 atoms, which is split in the case of TbAg$_3$In$_3$, whereas splitting is not observed by either structure determination method for the DyAg$_3$In$_3$ compound. The powder diffraction analysis yielded a site occupancy less than 1 for DyAg$_3$In$_3$. Finally, an additional atom site was located based on the X-ray powder analysis: Ag8 in Wyckoff position 12d with occupancy factor 0.29.

The refinement of the crystal structure resulted in the composition DyAg$_{3.010}$In$_3$ for the powder diffraction data and DyAg$_{2.853}$In$_3$ for the single crystal data. The small deficiency in silver atoms found for the single crystal led to lower values of the cell parameters. Interatomic distances and coordination numbers of the atoms are presented in Table 4.
Table 3 Anisotropic displacement parameters (Å$^2$) for DyAg$_{3.010}$In$_3$ (synchrotron X-ray powder diffraction) and DyAg$_{2.853}$In$_3$ (conventional X-ray single crystal diffraction).

<table>
<thead>
<tr>
<th>Atom</th>
<th>$B_{11}$</th>
<th>$B_{22}$</th>
<th>$B_{33}$</th>
<th>$B_{12}$</th>
<th>$B_{13}$</th>
<th>$B_{23}$</th>
</tr>
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<tbody>
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<td>Dy</td>
<td>0.49(15)</td>
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<td>0.3(2)</td>
<td>0</td>
<td>0</td>
<td>-0.17(13)</td>
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<tr>
<td>Ag1,2</td>
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<td>2.32(15)</td>
<td>2.32(15)</td>
<td>0.4(2)</td>
<td>0.4(2)</td>
<td>0.4(2)</td>
</tr>
<tr>
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<td>1.5(4)</td>
<td>0.9(4)</td>
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<td>0.4(3)</td>
</tr>
<tr>
<td>Ag6</td>
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<td>1.4(4)</td>
<td>2.0(4)</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Ag7</td>
<td>1.0(4)</td>
<td>1.5(4)</td>
<td>1.5(4)</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>In1</td>
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<td>1.4(3)</td>
<td>1.9(3)</td>
<td>0</td>
<td>0</td>
<td>-0.4(2)</td>
</tr>
<tr>
<td>In2</td>
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<td>1.9(2)</td>
<td>1.5(2)</td>
<td>0.3(2)</td>
<td>-0.19(14)</td>
<td>-0.3(2)</td>
</tr>
<tr>
<td>Dy</td>
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<td>Ag1,2</td>
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<td>1.87(6)</td>
<td>1.87(6)</td>
<td>1.29(8)</td>
<td>1.29(8)</td>
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<tr>
<td>Ag3,4</td>
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<td>In2</td>
<td>1.46(6)</td>
<td>2.38(7)</td>
<td>1.37(5)</td>
<td>0.60(5)</td>
<td>-0.35(5)</td>
<td>-0.43(5)</td>
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Fig. 1 Observed (circles), calculated (solid line) and difference diffraction patterns of the Dy$_{15}$Ag$_{43}$In$_{42}$ alloy: 1 – DyAg$_{3.010}$In$_3$; 2 – DyIn$_3$; 3 – Ag$_7$In$_3$. Synchrotron radiation, $\lambda = 0.49063$ Å.

The interatomic distances Ag-Ag within the coordination polyhedra range from 2.46 Å (Ag4-Ag5) to 3.19 Å (Ag6-Ag7), i.e. approximately 11 % less and more than the sum of the atomic radii, respectively. The shortest distance In-In is 2.86 Å (In2-In2) and the longest one is 3.56 Å (In2-In2), i.e. also 10-12 % less and more than the sum of the atomic radii [26]. The coordination polyhedra of the Dy atoms (CN = 16) is a pentagonal prism with additional atoms capping all of the lateral faces and one base. The coordination numbers of the Ag atoms are 10 for Ag1-Ag4, 7 for Ag5, 12 for Ag6, and 11 for Ag7, and correspond to coordination polyhedra in the form of trigonal prisms and derivatives of icosahedrons. The indium atoms have slightly higher coordination numbers, 12 for In1 and In2 (Fig. 2).

4. Conclusions

Quasicrystals are extremely sensitive to different external influences (e.g. temperature). In the YbCd$_6$ compound, one of the Cd atoms (Cd2) occupies the position 24g with occupancy 1/3 at 90 K, but 48h with
Table 4 Interatomic distances (δ, Å) and coordination numbers (CN) of the atoms in DyAg₂₆₅ ln₃.

<table>
<thead>
<tr>
<th>Atom</th>
<th>δ, Å</th>
<th>CN</th>
<th>Atom</th>
<th>δ, Å</th>
<th>CN</th>
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Fig. 2 Projection of the crystal structure of DyAg₂₆₅ ln₃ and the coordination polyhedra of the atoms (from X-ray single crystal diffraction data).
occupancy 1/6 at 240 K [27]. Similar changes are observed for other \(\text{RECd}_6\) compounds, especially when \(\text{RE} = \text{Pr}, \text{Eu}\). In this case both the splitting of the atomic positions and their occupancies change [28]. Similar differences exist between the structures of \(\text{YbAg}_2\text{In}_4\) [12], \(\text{TbAg}_3\text{In}_3\) [19] and \(\text{DyAg}_{2.853}\text{In}_3\) (or \(\text{DyAg}_{3.010}\text{In}_3\)), although the basic structural motif remains unchanged.

References


