# **Summary of Professional Accomplishments**

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1. Education and academic degrees	2
2. Information on employment in scientific units	2
3. Description of the achievements, set out in art. 219 para 1 point 2 of the Act	3
3.1. Title of the scientific achievements	3
3.2. List of publications constituting the scientific achievements	3
3.3. Description of the achievements	4
4. Information on scientific activity in national and international institutions	27
5. Information about the achievements in teaching, organization and popularizing	
science or art	29
6. Other information - development of measurement instruments and methods	30
7. Bibliography	31

# 1. Education and academic degrees

2002 – 2008 Polish Academy of Sciences, Institute of Physcics in Warsaw Scientific degree: **PhD in physics** Dissertation title: *Temperature and pressure dependence of structural properties of selected nitrides of group III and IV elements*. Thesis supervisor: prof. dr hab. Wojciech Paszkowicz

1997-2001 Donetsk National University, Donetsk, Ukraine Scientific degree: **specialist** (**Master**) Praca magisterska: *Effect of irradiation of fullerite coatings on the corrosion properties of titanium* Supervisor: PhD Antonina Trotsan

# 2. Informacje o dotychczasowym zatrudnieniu w jednostkach naukowych

16.11.2001 - 08.09.2002 Donetsk National University, Donetsk, Ukraine
Position: engineer
01.10.2002 - 01.10.2007 Polish Academy of Sciences, Institute of Physics in Warsaw
Position: PhD student
01.10.2008 - 31.03.2008 Polish Academy of Sciences, Institute of Physics in Warsaw
Position: assistant
15.07.2008 - 01.11.2011 Polish Academy of Sciences, Institute of Physics in Warsaw
Position: adjunct
01.11.2010 - 01.11.2011 Synchrotron in Trieste (Elettra), Italy
Research internship under the CERES (CEI) programme
02.11.2011 - 14.07.2014 Polish Academy of Sciences, Institute of Physics in Warsaw
Position: adjunct
15.07.2014 – 30.06.2024 Polish Academy of Sciences, Institute of Physics in Warsaw
Position: assistant
01.07.2024 – up to now Polish Academy of Sciences, Institute of Physics in Warsaw
Position: adjunct

# 3. Description of the achievements, set out in art. 219 para 1 point 2 of the Act

# **3.1.** Title of the scientific achievements

Thermostructural properties of selected semiconductors and functional oxides.

## 3.2. List of publications constituting the scientific achievements

**H1.** <u>Minikayev, R.</u>; Safari, F.; Katrusiak, A.; Szuszkiewicz, W.; Szczerbakow, A.; Bell, A.; Dynowska, E.; Paszkowicz, W. Thermostructural and Elastic Properties of PbTe and Pb<sub>0.884</sub>Cd<sub>0.116</sub>Te: A Combined low-temperature and high-pressure X-ray diffraction study of Cd-substitution effects, *Crystals* **2021**, *11*(*9*), an1063

**H2**. <u>Minikayev, R.</u>; Dynowska, E.; Kamińska, E.; Szczerbakow, A.; Trots, D.; Story, T.; Szuszkiewicz, W. Evolution of  $Pb_{1-x}Cd_xTe$  solid solution structure at high temperatures, *Acta Physica Polonica A* **2011**, *119*, 699

**H3**. <u>Minikayev, R.</u>; Dynowska, E.; Witkowska, B.; Bell, A.M.T.; Szuszkiewicz, W. Unit-cell dimensions of  $\alpha$ -MnTe in the 295 K – 1200 K temperature range. *X-Ray Spectrometry* **2015**, 44(5), 394

**H4.** Prokhorov, A.A.; Chernush, L.F.; <u>Minikayev, R.</u>; Mazur, A.S.; Zajarniuk, T.; Szewczyk, A.; Dyakonov, V;. Lančok, J.; Prokhorov, A.D. Structural and magnetic properties of  $YAl_3B_4O_{12}$  and  $EuAl_3B_4O_{12}$  single crystals doped with Co<sup>2+</sup>, *Journal of Alloys and Compounds* **2018**, 765, 710

**H5**. Prokhorov, A.A.; Chernush, L.F.; Melnik, T.N.; <u>Minikayev, R.</u>; Mazur, A.; Babin, V.; Nikl, M.; Lančok, J.; Prokhorov, A.D. Optical and magnetic properties of the ground state of  $Cr^{3+}$  doping ions in REM<sub>3</sub>(BO<sub>3</sub>)<sub>4</sub> single crystals, *Scientific Reports* **2019**, *9*, an12787

**H6**. Prokhorov, A.A.; Zubov, E.; Chernush, L.F.; <u>Minikayev, R.</u>; Babin, V.; Nikl, M.; Zajarniuk, T.; Szewczyk, A.; Savchenko, D.; Lančok, J.; Prokhorov, A.D. Comparative study of structural, optical and magnetic properties of Er<sup>3+</sup> doped yttrium gallium borates, *Results in Physics* **2020**, *19*, 103247

**H7**. Prokhorov, A.A.; <u>Minikayev, R.</u>; Savchenko, D.V.; Lančok, J.; Prokhorov A.D. Comparative study of structural and magnetic properties of the Tb<sup>3+</sup> ion doped into aluminum and gallium borate single crystals, *Materials Chemistry and Physics* **2022**, *275*, an125251

# **3.3.** Description of the achievements

## Introduction

Crystalline semiconductors and functional oxides are currently used to manufacture most of the electronic devices used by mankind. The search for new materials that have physical properties relevant to electronic applications and the modification of currently known materials is one of the main goals of scientific research in solid state physics. Regardless of other desirable characteristics, the basis for evaluating the possibilities and technical limitations of using such materials in electronic devices and developing new methods for obtaining these materials are their thermostructural properties, which describe the dependence of the materials' structure on external factors, such as temperature or pressure. Thermostructural properties such as thermal expansion, compressibility and structural stability are also of key importance in the design of electronic devices as they influence the growth processes of crystals and thin films and are important in predicting the behavior of the material under mechanical or thermal stress [1].

Non-destructive methods based on the phenomena of diffraction, absorption or other interactions of electromagnetic wave beams with matter, which can be applied by placing the material under study in conditions that differ from normal conditions, play an important role in structural research. One such method is X-ray powder diffraction, which allows precise determination of the structural features of a material, namely phase composition, type and dimensions of the elementary cell, position of atoms in the cell, positional occupancy by atoms, and thermal vibrations. By recording and analyzing such data under high and low temperature and high pressure conditions, we are able to determine the thermostructural properties of the material under study. Most of the results described in this thesis were obtained using the above method.

One of the materials that exhibit good thermoelectric properties are IV-VI semiconductors with a rock salt type structure. The family of thermoelectric materials includes tellurides, selenides, sulfides and some other compounds [2]. One of the most important thermoelectric materials in the family of Pb and Sn chalcogenides with rock salt structure is PbTe (alltaite). An effective way to modify the physical properties of these materials is to substitute specific elements (dopants) in the cationic or anionic sites of the crystal lattice using a synthesis method that preserves the original structure of the substituted material. Careful selection of the dopant and its amount in the PbTe lattice can significantly increase the Seebeck coefficient [3,4]. The solubility limit of the selected dopant in the analyzed material depends on both the specific element and the method used to obtain such a material.

Detailed studies to analyze the dependence of the crystalline structure of the material on the applied pressure and temperature in a wide range of variation of these parameters were not available for solid solutions of type II-VI and IV-VI semiconductors. This fact was the motivation for the investigation of  $Pb_{1-x}Cd_xTe$ , one of the most studied thermoelectric materials. Solid solutions of  $Pb_{1-x}Cd_xTe$  are a promising material for the fabrication of thermoelectric modules operating in the medium temperature range [5]. Due to the isoelectronic effect of the cadmium atoms in lead telluride, both p-type and n-type elements for thermoelectric junctions can be fabricated from this material [6]. Thin films fabricated on the basis of  $Pb_{1-x}Cd_xTe$  can also be used for the development of flexible miniature devices such as thermoelectric micromodules [7,8].

Another group of materials of interest from the point of view of applications are diluted magnetic semiconductors (DMS). These materials, also known as semi-magnetic semiconductors, were intensively studied in Poland for a number of years. Nowadays, the idea of using them in spintronic

devices has rekindled interest in such materials, since some of them exhibit magnetic properties under normal conditions. Among the binary manganese compounds,  $\alpha$ -MnTe is of particular interest to researchers because of the presence of antiferromagnetic ordering observed at temperatures slightly above room temperature. The  $\alpha$ -MnTe compound has a NiAs-like hexagonal structure [9]. The crystal structure of this compound is stable at room temperature as well as over a wide range of high temperatures (up to 1222 K) [10]. This material is characterized by a relatively high Néel temperature (about 310 K) [11], and for thin films obtained by the MBE method on sapphire substrates it is even several degrees lower [12]. The development of the technology for growing  $\alpha$ -MnTe thin films by the MBE method has opened up the possibility of using this material as a component of multilayer systems.

The high-temperature modifications of this compound -  $\beta$ -MnTe with a zinc blende structure,  $\gamma$ -MnTe with a wurtzite structure, and  $\delta$ -MnTe with a rock salt structure - can exist under thermodynamic equilibrium conditions only in a very narrow temperature range [10]. Of the three high-temperature phases, the zinc-blende-structured crystal modification ( $\beta$ -MnTe), which exhibits antiferromagnetic ordering, is the best known because of its role as a component of many important DMSs [13]. In recent years, the  $\beta$ -MnTe compound has also been considered as a promising material for making contacts in CdTe-based thin-film photovoltaic solar cells [14], where alternative copper-free back contacts are needed [15].

Completely new prospects for the practical application of  $\alpha$ -MnTe and other similar compounds are opened by recent studies [16] conducted on this compound and confirming the existence of a hitherto theoretically predicted class of materials under the name "altermagnetics" [17], i.e., materials that behave as ferromagnets in *k*-space, while in real space they behave as antiferromagnets (with zero resultant magnetization). Since altermagnetic properties occur only in non-cubic MnTe crystals and are associated with the antiferromagnetic phase transition, precise studies of the thermostructural properties of these materials are essential.

Other promising materials with a wide range of potential applications are multicomponent systems of aluminum and gallium borates with rare earth elements.  $RM_3(BO_3)_4$  crystals with a huntite structure, where R is rare earth or yttrium ions and M is Al, Fe, Ga, Sc or Cr, have recently been actively studied for various physical properties. Borates have high rare earth solubility, high melting points, and are moisture resistant, making these crystals suitable matrices for lasers [18,19], scintillators [20], phosphors [21,22], and other optical devices [23-28]. The near-infrared (NIR) and VIS emission of borate glasses doped with rare earth elements makes them very attractive materials for laser applications. In recent years, interest in REE-doped borate glasses has grown rapidly [23-27] due to their impact on the development of new luminescent and optical materials. Recently, stringent requirements have been formulated for practical nonlinear optical (NLO) materials in the ultraviolet (UV) and deep ultraviolet regions [27]. These materials should: (1) crystallize into an effective class of non-centrosymmetric crystals; (2) have high transparency in the UV spectral region with short cutoffs in the deep UV; (3) exhibit high second-order NLO coefficients; (4) have sufficient birefringence to achieve phase matching conditions in the UV and deep UV; (5) have a high laser destruction threshold with reasonable chemical stability; (6) be able to easily form a single crystal of large size. According to these requirements, borate crystals can be suitable candidates for UV and deep-UV NLO devices because they can form non-centrosymmetric structures, have wide windows of optical transparency (due to the large difference in electronegativity between boron (B) and oxygen (O) atoms), and high polarization leading to the coexistence of suitable NLO coefficients [27].

The prospects for widespread practical application of the three groups of materials mentioned above, coupled with the rather limited, or sometimes lack of, knowledge of selected aspects of their thermostructural properties, motivated me to undertake detailed structural and thermostructural studies of these materials.

# Study of the effect of Cd substitution in place of Pb in PbTe on the thermostructural and elastic properties of the resulting solid solution

Experimental and theoretical studies on the effect of substitution of parent atoms in semiconductor compounds by foreign atoms on the structural and elastic properties of PbTe are widely reported in the literature. For example, for PbTe crystals modified by doping with various elements, studies have been carried out for elements such as Ba [29], Cd or Mn [30], gold [33], rare earth metals [31], and a number of other elements [32]. According to theoretical considerations [32], the Debye temperature and the Seebeck coefficient change for most of the dopants shown. Predicting the value of the Seebeck coefficient and the Debye temperature provides valuable guidance for future work to improve the thermoelectricity of materials. Thus, the thermoelectric properties of PbTe are improved when Pb ions are partially replaced by Cd ions [34] to form a metastable  $Pb_{1-x}Cd_xTe$  solid solution that retains a rock salt-like structure [35-38]. This material, which is suitable for the design of thermoelectric devices, has attracted the attention of researchers.

The lattice parameter of  $Pb_{1-x}Cd_xTe$  decreases linearly with the addition of CdTe [39-42]. This behavior is similar to that of PbSe and PbS crystals with corresponding additions of CdSe [43-46] and CdS [47-50]. The highest reported cadmium content (*x*) for the (Pb,Cd)Te system is 0.75 [41], for (Pb,Cd)Se – 0.26 [43] and 0.4 for (Pb,Cd)S [48].

Many of the studies of the thermostructural and elastic properties of PbTe have not been very detailed, and even fewer have covered the lowest temperatures (below 105 K), especially those obtained using X-ray diffraction. The most detailed work is that of [51], that used neutron powder diffraction to determine changes in lattice parameters and mean square displacements (MSD) of atoms as a function of temperature. From these data, the thermal expansion coefficient (TEC) and the Debye temperature were determined. Other experimental work covers a narrower temperature range or describes only selected variables. Basic thermostructural data for the PbTe system, such as the lattice parameter a(T), are described in papers based on experimental results in refs. [51,53,58-63] and theoretical results in refs. [66-71], atomic shifts (experimental data ref. [51,53,56,59-63,71,76-78] and theoretical data ref. [61,70,71,79-81]) as well as thermal expansion a(T) (experimental data ref. [51,63,72,73] and theoretical data ref. [31,66-68,74,75]). Another frequently considered property of thermoelectric materials is the degree of order of the atoms [52]. Some recent studies have focused on the occurrence of disorder in the cation subnetwork in PbTe and related chalcogenides [53-56], which can affect the thermal conductivity of the crystal [53]. The disorder resulting from the substitution of Pb by Cd in the solid solution of (Pb,Cd)Te has recently been discussed in a paper [57].

As for the properties of PbTe that describe the behavior of its crystalline structure under pressure, or describe it in the space of the two variables p and T, or describe the changes in compressibility, elastic constants, heat capacity, Debye temperature and Grüneisen parameter as a function of temperature or pressure, the available data were very sparse. Experimental data for PbTe can be found in papers [31,72,73,82-84], theoretical data in papers [31,66-68,74,85-90] and for Pb<sub>1-x</sub>Cd<sub>x</sub>Te in papers [87,89].

The phase diagram of the Pb-Te system as a function of temperature shows that the Fm-3m phase of PbTe (with lattice parameter a = 6.460 Å) is stable over the whole temperature range up to  $T_{\text{max}} = 1197$ K [91] (see also ref. [92,93]). The range of non-stoichiometry for PbTe is very narrow [91,94-97]. The PbTe-CdTe phase diagram [36] (for theoretical considerations see ref. [87]) shows that the solubility of CdTe in PbTe under equilibrium conditions at room temperature is marginal. This is due to the difference in the crystal structure of the two compounds - PbTe is a salt type structure, CdTe is a zinc blende type structure. A solid solution of  $Pb_{1,r}Cd_rTe$  of the table salt type can be obtained in a metastable form. The results of such studies made it possible to estimate the maximum possible Cd content in the metastable solid solution [36]. Diffraction studies of the structure of  $Pb_{1,x}Cd_xTe$  at high temperatures, performed with my participation, have shown the process of metastable decomposition of Pb<sub>0.904</sub>Cd<sub>0.096</sub>Te already above 300 K [H2] (details of this work are described below). Experimental and theoretical studies of the high-pressure behavior of PbTe show that the transition to the highpressure polymorph occurs at a pressure of about 6-7 GPa (experimental data [91,98-104], theoretical data [88,105,106]). The space group of the polymorph is *Pnma*, the lattice parameters at 7.5 GPa are a = 11.91 Å, b = 4.20 Å, c = 4.51 Å [91]. From a pressure range of about 18 GPa to at least 50 GPa there is a phase with a CsCl-like structure [104]. In addition, density functional theory studies have reported a topological phase transition at 4.8 GPa [107].

As you can see, thermostructural experimental data on the behavior of the (Pb,Cd)Te system under different temperature and pressure conditions were not available before. A few data on the behavior of the lattice parameter have been published by me in a few conference papers [64,65]. In other words, taking into account the above, the purpose of the research I performed was to systematically determine the effect of cadmium substitution on the thermostructural and elastic properties of pure PbTe and Pb<sub>1-x</sub>Cd<sub>x</sub>Te.

For this purpose, the lattice parameter, thermal expansion, thermal shifts of atoms, bulk modulus and their variation with temperature or pressure have been studied and compared for crystals PbTe and Pb<sub>0.884</sub>Cd<sub>0.116</sub>Te and Pb<sub>0.904</sub>Cd<sub>0.096</sub>Te obtained by the self-selecting vapour phase growth (SSVG) method [108,109,110]. The Cd content, x = 0.116, is the highest content obtained for a given material. Temperature in-situ techniques using synchrotron radiation (temperature range 15-300 K and 300-1100 K) were used to perform the studies included in this dissertation [111]. Structural analysis of the obtained data was performed using the Rietveld method [113,114]. Examples of graphical results of crystal structure refinement for PbTe and Pb<sub>1-x</sub>Cd<sub>x</sub>Te samples at temperatures of 15 K, 300 K and 713 K are shown in Figures 1 and 4. Studies under high pressure conditions (in the pressure range of 0.1 MPa - 4.5 GPa.) were performed by the group of Professor Katrusiak of Adam Mickiewicz University in Poznan. They used a Merrill-Bassett diamond anvil chamber (DAC) for the measurements [115], and determined the crystal structure parameters by direct methods and refined them by the methods described in references [116,117]. However, I carried out the direct analysis of these results for the determination of the bulk modulus and its variation with pressure directly.



Figure 1 Graphical results of the crystal structure refinement of  $Pb_{1-x}Cd_xTe$  by the Rietveld method [H1]. Red dots - experimental data, black line - calculated result, vertical green bars - positions of Bragg peaks of  $Pb_{1-x}Cd_xTe$  (top) and internal reference material [112]- diamond (bottom), solid blue line - difference between experimental data and model predictions.

The obtained experimental lattice parameters of PbTe and Pb<sub>0.884</sub>Cd<sub>0.116</sub>Te in the range of 15-300 K will change monotonically (see Figure 2a). For PbTe, the lattice parameter increases by 0.50% over the entire temperature range. The a(T) run is marginally different from recent experimental data obtained over a wide temperature range (10-500 K) by neutron powder diffraction [51], and in the 105-300 K range by X-ray powder diffraction [53] (Figure 2a). A comparison based on this figure and the experimental values near 0 K (data from refs. [51,46]) and near 300 K (data from refs. [49,51,53,56,61,63-64,H2]), shows that the discrepancies between the lattice parameter values I obtained and the literature values are quite small. Near 0 K, the discrepancy of the obtained value, 6.42972(5) Å from the literature data, 6.42962 Å, is negligible (1×10-4 Å). At 300 K, the present result of fitting the experimental data is 6.46148(87) Å [H1]. It agrees perfectly with the average of the high-quality measurements for PbTe posted in the ICSD database [28] which is 6.46148(15) Å after temperature correction from 293 K (the temperature reported in the database) to 300 K. All these excellent matches indicate both the high quality of the sample and the precision of the measurement method used, including the calibration of the instrument.



Figure 2. Experimental temperature dependence of the lattice parameter (a) and the change of the normalized unit cell volume with temperature (b) for PbTe ( $\Box$ ) and Pb<sub>0.884</sub>Cd<sub>0.116</sub>Te ( $\Box$ ) in the low temperature range [H1]. In both cases the second order Grüneisen approximation fits are shown in the figure with red lines for PbTe and blue lines for Pb0.884Cd0.116Te. Literature experimental data for the lattice parameter PbTe are taken from ref. [60] ( $\triangle$ ), ref. [53] ( $\Box$ ), ref. [51] (black dashed line), ref. [61] ( $\diamond$ ), ref. [56] ( $\bigcirc$ ).

The temperature dependence of the values of the parameter a(T) obtained by me and reported in the literature is in line with previous theoretical results, and their absolute values differ only in the range of 0.3% 0.3% [67] to 2% [66]. The best fit to the present results, the increase in a in the range 15-300 K is slightly larger than experimentally determined (see H1 for details). The change in elementary cell volume with temperature, V(T), was modeled using the second-order Grüneisen approximation, taking into account the Debye internal energy function [119,120]. The fitted Grüneisen equation perfectly describes the experimental runs for both crystals, as shown in Figure 2b. Based on these results, the lattice parameter curves for both crystals were also determined.

The lattice parameter of Pb<sub>0.884</sub>Cd<sub>0.116</sub>Te (Figure 2a) is reduced relative to that of pure PbTe over the entire temperature range. The increase in the parameter *a* over the entire range of temperatures studied is apparently larger than for PbTe, at 0.53%. According to the model fitted to the experimental data, the lattice parameter for Pb<sub>0.884</sub>Cd<sub>0.116</sub>Te, increases from 6.37725(6) Å to 6.41133(116) Å. The difference from PbTe in the slope of the cell size-temperature dependence is shown in Figure 2a.Comparing the present result with previous results for lower Cd contents [64-65, H2] it can be deduced that the course of *a*(*T*) for the (Pb,Cd)Te crystal depends on the amount of substituent. A similar effect of the substituent on the *a*(*T*) waveform is also observed for PbTe crystals substituted with nickel and europium [63].

At high temperatures, above room temperature, a strong nonlinear evolution of the crystal lattice parameters is observed [H2]. Figure 3 shows such an evolution for a solid solution of  $Pb_{0.944}Cd_{0.056}Te$ . The reason for this behavior is the change in the content substituent in the PbTe matrix with temperature. In the temperature range from 295 K to about 500 K, the nature of the temperature

evolution of the lattice parameter values determined for the (Pb,Cd)Te sample is quite similar to the behavior of pure PbTe. Above 500 K, the Pb<sub>0.944</sub>Cd<sub>0.056</sub>Te solid solution tested changes its chemical composition, and the Cd content decreases to a composition slightly below x = 0.01 at about 700 K. This value is analogous to the result given in ref. [121]. It can be said that the studied metastable system Pb<sub>1-x</sub>Cd<sub>x</sub>Te has reached thermodynamic equilibrium at this temperature. On the diffraction patterns obtained in this temperature range (Figure 4), the absence of the diffraction signal of cadmium in crystalline form is observed. This probably indicates that Cd is still present in the sample, but in the form of nanoclusters or small liquid droplets, which cannot be detected using diffraction techniques. It should also be noted that the melting point for pure cadmium is  $T_{\rm m} = 594$  K, but for cadmium in the form of nanoclusters this temperature is much lower. At temperatures above 700 K, recrystallization of (Pb,Cd)Te occurs, which is characterized by a decrease in the lattice parameter of the (Pb,Cd)Te solid solution and a significant increase in the Cd content. Finally, all the Cd returns to the crystalline phase and a homogeneous solid solution of Pb<sub>0.944</sub>Cd<sub>0.056</sub>Te is formed, and the evolution of the lattice parameter again becomes similar to that of pure PbTe (Figure 3). Such a change in Cd content of the PbTe matrix with temperature has not been reported in the literature. The method of investigation shown can be considered as a method for completing the phase diagrams of metastable systems.



Figure 3. Experimental high-temperature dependence of the lattice parameter for PbTe ( $\Box$ ) and Pb<sub>0.944</sub>Cd<sub>0.56</sub>Te ( $\Box$ ) [H2].

Figure 4: Graphical results of Pb<sub>0.944</sub>Cd<sub>0.056</sub>Te structure refinement by Rietveld method [H2]. Red dots - experimental data, black line - model pattern, vertical green bars - positions of Bragg peaks (Pb,Cd)Te (top) and internal standard [112]-diamond (bottom), continuous blue line - difference between experimental data and model.

The experimental dependence of the coefficient of linear thermal expansion on temperature, a(T), was derived from the Grüneisen V(T) approximation using the equation:  $\alpha(T) = \alpha_V(T)/3 = (dV/dT)/(3V(T))$ . The general nature of the changes in  $\alpha(T)$  is typical for both materials. At the lowest temperatures (from 0 to 10 K) its value is almost constant. A pronounced increase is observed from 10 K to about 100 K, and above this temperature the increase gradually weakens significantly. In the range from about 170 K to room temperature, the change of  $\alpha$  with temperature is weak and almost linear (Figure 5a) The obtained temperature dependence of the expansion coefficient for PbTe shows good

agreement with experimental results obtained by neutron powder diffraction techniques [51] and dilatometry [72] (Figure 5b). In particular, the experimental value of the expansion coefficient (19.6(6)  $MK^{-1}$ ) obtained by me for a temperature of 300 K differs by only 1.5% from the previously reported experimental values of 19.80  $MK^{-1}$  [72] and 19.91  $MK^{-1}$  [51].



Figure 5: Variability of thermal expansion with temperature,  $\alpha$ (T) [H1]. (a) For PbTe and Pb<sub>0.884</sub>Cd<sub>0.116</sub>Te as a function of temperature. (b) Comparison of the present data for PbTe (red solid line) with literature experimental data (ref. [72] - •, [51] - black dashed line) and theoretical PbTe (ref. [67] - ×, ref. [31] - **O** and ref. [71,122] – heavily overlapping with red line - turquoise dotted line).

I also observed a remarkable agreement of the obtained experimental data on the thermal expansion of PbTe with the theoretical data reported in refs. [71,122]. Dla innych danych teoretycznych trendy tych wyników są generalnie zgodne z eksperymentami opisanymi tutaj i innych pracach. ]. For other theoretical data, the trends of these results are generally consistent with the experiments described here and in other papers. In particular, the present data differ only slightly from the theoretical data of ref. [67] up to 100 K, while the discrepancy increases significantly at higher temperatures. The increase in the coefficient of thermal expansion,  $\alpha(T)$ , for Pb<sub>0.884</sub>Cd<sub>0.116</sub>Te over the temperature range studied is more pronounced than for PbTe (Figure 5a). At 300 K the coefficient is about 6.5% higher than for PbTe, reaching a value of 20.7(8) MK<sup>-1</sup>, while at the lowest temperatures the increase is comparable.

The mean-square isotropic atomic displacement,  $\langle u^2 \rangle$ , for the cations and anions PbTe and Pb<sub>0.884</sub>Cd<sub>0.116</sub>Te monotonically increase with increasing temperature (Figure 6). This dependence can be modeled as shown in ref. [124] using the equation:  $\langle u^2 \rangle (T) = \langle u^2 \rangle_{dyn}(T) + \langle u^2 \rangle_{stat}$ , which takes into account the temperature-dependent dynamic disorder component  $\langle u^2 \rangle_{dyn}(T)$  modeled by the Debye function [123] (based on a simplified assumption that takes acoustic branches into account, while it ignores optical branches) and the temperature-independent static disorder component  $\langle u^2 \rangle_{stat}$  which is the empirical term assigned to the temperature-independent static disorder. This term in unsubstituted crystals can be related, for example, to point defects [125], the presence of which affects the electrical and other properties of thermoelectric crystals [126], while in substituted crystals it can be related to the presence of foreign atoms in cationic or anionic sites.



Figure 6: Temperature dependence of mean square displacement for cations (a) and anions (b), for PbTe ( $\Box$ ) and Pb<sub>0.884</sub>Cd<sub>0.116</sub>Te ( $\Box$ ) [H1].Red and blue solid lines represent fitted Debye functions.

In general, the run of the  $\langle u^2 \rangle(T)$  curve representing either a cationic or anionic site shows a characteristic linear dependence at higher temperatures, having a definite slope, and static behavior at the lowest temperatures. The basic parameters describing a given dependence are the atomic mass of the elements in the crystal, *m*, the Debye temperature,  $\theta_D$ , and the disorder parameter,  $\langle u^2 \rangle_{\text{stat}}$ .

Analysis of the obtained dependencies (Figure 6) shows that the fitted  $\langle u^2 \rangle$ (T) curves for PbTe and  $Pb_{0.884}Cd_{0.116}Te$  behave differently. The MSD value at temperature 0 K,  $\langle u^2 \rangle (T = 0)$ , increases significantly (by about 0.002-0.004  $Å^2$ ) as x increases from 0 to 0.116. This increase can be prescribed by the appearance of static disorder, expressed by obtaining a non-zero value of the  $\langle u^2 \rangle_{\text{stat}}$  term. For a mixed crystal relative to a PbTe crystal, an increase in the static disorder component,  $\langle u^2 \rangle_{\text{stat}}$ , is observed from  $0.38(4) \times 10^{-3} \text{ Å}^2$  to  $2.03(6) \times 10^{-3} \text{ Å}^2$  for cations and from  $-0.54(7) \times 10^{-3} \text{ Å}^2$  to  $3.4(1) \times 10^{-3} \text{ Å}^2$  $10^{-3}$  Å<sup>2</sup> for anions. At higher temperatures, the cationic MSDs are almost the same for both crystals, while the anionic MSDs differ significantly over the entire temperature range. The slope of the cationic  $\langle u^2 \rangle$  (T) curve decreases with increasing x, while the anionic curve appears to increase. The slope of the function  $\langle u^2 \rangle$ (T) is dependent at high temperatures on the Debye temperature (for a large slope, the Debye temperature is low and vice versa). MSDs for cationic and anionic positions behave differently for x = 0 than for x = 0.116. Cationic and anionic MSDs for Pb<sub>0.884</sub>Cd<sub>0.116</sub>Te have comparable values in the temperature range studied. Since this effect must depend on x, we expect that for x<0.116 the  $\langle u^2 \rangle$  values of the anions will be lower than those of the cations, while for x>0.116 (when the structure is stabilized) the values for the anions will be higher. The observed increase in  $\langle u^2 \rangle_{\text{stat}}$  values after the introduction of Cd into the PbTe lattice is evidence that the formation of the alloy causes the appearance of substituent disorder in the mixed crystal. The disorder in the anion subnetwork is much higher in this crystal. The obtained results on disorder for both subnetworks, cationic and anionic, in the PbTe-based mixed crystal are an important novelty. Analysis of this kind will be useful in future studies of solid solutions of type IV-VI thermoelectric semiconductors. Disorder in solid solutions is important for applications of these materials because it can affect carrier mobility, electrical conductivity [54,57] and thermal conductivity [53,131] by affecting the Seebeck coefficient.

Comparison of the determined MSDs for PbTe with literature data indicates their similarity to neutron scattering-based data [51,60] and some other data based on X-ray diffraction [53,56,59] (see Figure 7). The different slopes of the quasi-linear parts of the experimental  $\langle u^2 \rangle (T)$  relationships may be related to differences in the defect structure of the monocrystals and polycrystals studied. A better fit above 50 K to the experimental results I obtained can be seen for data based on molecular dynamics calculations from ref. [61] and near 0 K for the theoretical data of refs. [79] and [80].



Figure 7. Temperature dependence of mean square displacement of cations (a) anions (b) in PbTe. (Red squares and red solid line [H1]). Literature experimental data: ref. [59] (O), ref. [60] ( $\triangle$ ), ref. [53] ( $\nabla$ ), ref. [56] ( $\bullet$ ), ref. [51] (black dashed line), ref. [61] (+) and teoretyczne: ref. [79] (×), ref. [61] (black dotted line).

An important thesis is the effect of substitution of Pb by Cd in the PbTe lattice on the change in cell dimensions and compressibility modulus with pressure. To determine it, I performed high-pressure insitu X-ray diffraction studies at pressures up to 4.5 GPa. The NaCl-type crystal structure found for PbTe and Pb<sub>0.884</sub>Cd<sub>0.116</sub>Te monocrystals under normal conditions (T = 295 K and P = 0.1 MPa) was preserved under the applied high-pressure conditions. Fitting the structure to the experimental data resulted in a lattice parameter that monotonically varies with increasing pressure. In the analysis, I used the Birch-Murnaghan equation of state (BMEOS) [118] of the second order, in which the function of the pressure P in an elementary cell from its volume depends on the parameter - the compressibility modulus K0 of the material. The equation assume Eulerian deformation between atoms and the derivative of the bulk modulus - K' was set equal to 4. The experimentally determined relative volume of the elementary cell as a function of pressure is well described by this equation (Figure 8a). The obtained value of the compressibility modulus for PbTe K0 is equal to 45.6(2.5) GPa, which is consistent with previously reported values, in particular with those obtained from X-ray diffraction studies: 38.9 GPa [99,101] and 44(1) GPa [104], as well as values from early ultrasonic wave velocity measurements ref. 41.26 GPa [51], 39.76 GPa [73], 40.5(7) GPa [84], 38.39 GPa [127]. The bulk modulus values reported in theoretical studies [33,66,67,85,128-131], mainly based on different density functional theory approximations, range from 38.54 GPa to 51.7 GPa.

The bulk modulus of  $Pb_{0.884}Cd_{0.116}$ Te at room temperature is 33.5(2.8) GPa [H1], providing the first experimental evidence that substitution of Pb by Cd reduces the stiffness of the PbTe matrix. For both

crystals, the bulk modulus increases with pressure, from 0.1 MPa to 4.5 GPa, by about 50% (Figure 8b). For PbTe, the K(p) relationship is consistent with the theoretical one reported in ref. [85].



Figure 8. Relative unit cell volume,  $V/V_0$ , as a function of pressure (a) and bulk volume modulus,  $K_0$ , as a function of pressure (b) for PbTe ( $\Box$ ) and Pb<sub>0.884</sub>Cd<sub>0.116</sub>Te ( $\Box$ )crystals (solid line - BMEOS fit) [H1]. Literature data for PbTe are experimental from ref. [104] (**O**)and fit (black dotted line), and theoretical from ref. [85] ( $\triangle$  and black dashed line).

There are a number of theoretical papers investigating changes in the bulk modulus following substitution of an element in the cationic site [31,32,132] - the most common prediction is that it will decrease. In ref. [32], the value of the bulk modulus was calculated for 62 elements partially substituting Pb in PbTe. The same calculations were carried out for nine substituents in the anionic Te site. For almost all of them the bulk modulus decreases, while for V, Nb, Ni and Bi the  $K_0$  value is greater than the calculated value of 46.61 GPa [32] for pure PbTe. The reference [32] predicts that  $K_0$ decreases from 46.61 GPa for PbTe to 46.42 GPa for Pb<sub>0.969</sub>Cd<sub>0.031</sub>Te. This leads to an extrapolated value of 45.90 GPa for Pb<sub>0.884</sub>Cd<sub>0.116</sub>Te. This evaluation differs from the experimental value obtained in this paper (33.5(2.8) GPa), but the direction of change of  $K_0$  with x is the same. Experimental values of  $K_0$  for PbTe substituted with any cation are not available, except in the case of Ba substitution where the effect of mixing on  $K_0$  is to reduce the value for PbTe by 5% [29]. The assumption that  $K_0$ (PbTe) is equal to 46.61 GPa leads to an estimate of the (not explicitly stated) experimental value, 44.3 GPa for Pb<sub>0.96</sub>Ba<sub>0.04</sub>Te. Extrapolation of the theoretical value of 44.99 GPa for Pb<sub>0.969</sub>Ba<sub>0.031</sub>Te given in ref. [32] leads to  $K_0 = 44.5$  GPa for Pb<sub>0.96</sub>Ba<sub>0.04</sub>Te. The excellent agreement between calculated values of 44.3 GPa and experimental values of 44.5 GPa indicates the reliability of both the cited experiment and calculations.

As for the determination of the Debye temperature,  $\theta_D$ , of the materials studied, this was made possible by modelling three relationships, V(T),  $\langle u^2 \rangle \langle T \rangle$  and V(P). In general,  $\theta_D$  is often considered as a temperature dependent quantity, but for PbTe the reported changes in  $\theta_D$  are weak and mainly observed at cryogenic temperatures [74,82]. In most studies, including those based on diffraction,  $\theta_D$  is considered to be a temperature independent quantity. For NaCl-structured compounds, different  $\theta_D$ values are reported for the cationic and anionic sublattices. Such a distinction is possible by matching the thermal atomic vibrations of a given sublattice (cationic or anionic) using the Debye equation. Consequently, from the study we obtain a single overall  $\theta_D$  value from the matching of V(T) and a pair of  $\theta_D$  from the matching of  $\langle u_C^2 \rangle(T)$  and  $\langle u_A^2 \rangle(T)$  (the respective symbols  $\theta_{DV}$ ,  $\theta_{DUC}$  and  $\theta_{DUA}$  are used here to emphasise the distinction between these three definitions of  $\theta_D$ ), while the overall  $\theta_{DU}$  denotes the average of  $\theta_{\text{DUC}}$  and  $\theta_{\text{DUA}}$ . The current total  $\theta_{\text{D}}$  values for PbTe ( $\theta_{\text{DV}}$  and  $\theta_{\text{DU}}$ ) are almost identical (135.2(3.8) K and 135.9(7) K; the average is ~135.5 K), and the Debye temperature for the cationic and anionic sublattices are  $\theta_{DUC} = 102.8(3)$  K and  $\theta_{DUA} = 169(1)$  K, respectively. The first PbTe diffraction studies showed a relatively low overall Debye temperature for PbTe, around 110 K [76,77]. The overall  $\theta_{\rm DV}$  and  $\theta_{\rm DV}$  values obtained for the PbTe lattices are in agreement with those obtained in ref. [51] (128(1) K) The present overall  $\theta_D$  values are also in line with the trends observed for values obtained by non-diffraction methods [36,73,82,84,133-139] (their mean calculated for data at room temperature is 138.1 K, which is only 3 K higher than the value obtained by the author of this work in [H1]). The application of theoretical methods [32,51,68,78,140,141]) resulted in values with a higher mean of 157.9 K; these data vary over a wide range. Experimental results (present and previous [51,53,63,76,77]) show that the values determined for cations by other research groups are in very good agreement (they have a value between 95.5 and 102.8 K), whereas the values determined for anions have a wider range between 127 and 169 K. With the substitution of Cd, a slight reduction of the total Debye temperature,  $\theta_{DU}$ , of 5.1 K is observed. Theoretical calculations predict a reduction of 2.4 K for a composition of x = 0.031 [32]. Extrapolation of this result to the composition of the mixed crystal studied in this work (x = 0.116) gives a prediction of a reduction of 9 K. This theoretical result supports the observed trend of lowering the overall Debye temperature by increasing the cadmium content. Interestingly, the  $\theta_D$  values given by different authors for the cationic sublattice are in almost perfect agreement, while a scatter is observed for the anionic sublattice. The observed effects of Cd substitution in the PbTe lattice on the investigated thermostructural and elastic properties can serve as a basis for evaluating these properties for crystals with different Cd contents. They may also be useful in the study of more complex systems, such as those with cationic-anionic double substituents. As noted in reference [52], several factors affect the value of the Seebeck coefficient. One way to optimise this value is to use an alloy with the chosen element. An equally possible solution is to use more complex systems where there are less conventional double substituted cationic systems such as Na<sub>0.03</sub>Eu<sub>0.03</sub>Pb<sub>0.94</sub>Te or cationic-anionic systems - Na<sub>0.03</sub>Eu<sub>0.03</sub>Pb<sub>0.94</sub>Te<sub>0.9</sub>Se<sub>0.1</sub> [126]or (Pb,Cu)(Se,Te) [142].

Using the relationships  $\alpha(T)$  and  $V_m(T)$  obtained for (Pb,Cd)Te, it was also possible to evaluate the variation of the Grüneisen parameter  $\gamma$  with temperature using the formula given in ref. [51]  $\gamma(T) = \alpha(T)K_0(T)V_m(T)/c_v(T)$ , where  $\alpha$  is the coefficient of thermal expansion,  $K_0$  is the bulk modulus and  $c_v$  describes the isochoric heat capacity. For this purpose, the variation of  $K_0(T)$  reported in ref. [51] for PbTe was scaled to the present  $K_0$  at room temperature obtained for both samples as PbTe so and Pb<sub>0.884</sub>Cd<sub>0.116</sub>Te. The temperature variation of the molar isochoric capacity  $c_v(T)$  for PbTe was taken from ref. [51], while for the Pb<sub>0.884</sub>Cd<sub>0.116</sub>Te sample the theoretical  $c_v(T)$  data for Pb<sub>0.88</sub>Cd<sub>0.12</sub>Te were used [89]. The correlations calculated on the basis of these assumptions are shown in Figure 9. The obtained values of  $\gamma(T)$  for PbTe are comparable with the value of about 1.5 given in ref. [72] in the range 30-340 K and with the values of about 2.1-2.2 in the range 50-260 K given in ref. [51].



Figure 9: Temperature variation of the Grüneisen parameter for PbTe and Pb<sub>0.884</sub>Cd<sub>0.116</sub>Te [H1].

The parameter  $\gamma$  is often treated as a constant. Its experimental constant value determined by the neutron diffraction method is 2.03 [51], while the sound velocity method gave a result of 0.95 [84], and the ultrasonic wave velocity method gave 1.96 [36]. The theoretical values obtained by density functional theory are 1.96-2.18 [66], while molecular dynamics gave  $\gamma = 1.66$  [131]. Interestingly, the present results and some of those concerning the  $\gamma$  constant consistently suggest that its value is close to 2, while roughly evaluated mixed crystal data indicate some reduction in  $\gamma$  as a result of Cd substitution. The reliability of the thesis author's calculated value of  $\gamma$  at the lowest temperatures depends on the accuracy of the  $\alpha$  and  $c_{\gamma}$  values, so the reduction in  $\gamma$  observed in the plots below ~50 K may be questioned.

#### Evolution of the $\alpha$ -MnTe unit cell at high temperatures.

As mentioned earlier, the thermostructural properties of materials are extremely important from the point of view of the technology for obtaining these materials in various forms or their applications. Due to new concepts of MnTe applications in semiconductor spintronic systems and, at the same time, the rather limited knowledge of the thermostructural parameters of  $\alpha$ -MnTe above room temperature, structural studies of this material at high temperatures have gained importance. The timeliness of such studies has also increased as a result of the recent discovery of the occurrence of an alltermagnetic effect in non-cubic MnTe crystals.

The objects of my research were  $\alpha$ -MnTe monocrystals grown at the Institute of Physics of the Polish Academy of Sciences in Warsaw using the vapour phase physical transport method [143]. The crystals were powdered and subjected to X-ray diffraction studies using equipment available in our laboratory and synchrotron radiation. High temperature in-situ measurements at temperatures from 295 K to 1200 K were performed at the synchrotron beamline B2 at Hasylab/DESY in Hamburg. For both data sets the Rietveld method was used to determine the lattice parameters at each temperature as well as the content and properties of the temperature induced phases. Graphical results of the refinements for the sample measured with synchrotron radiation at temperatures of 313 K and 623 K are shown in Figure 8.

Phase analysis of the obtained crystals showed that the studied material crystallized in a hexagonal structure of NiAs type (space group: P63/mmc) with the following values of lattice parameters: a = 4.14794(5) Å, c = 6.7118(1) Å, c/a = 1.61811(9) [H3]. The initial material does not have any additional minority crystalline phases. The determined lattice parameters and c/a ratio in the error range are in agreement with the data in ref. [144] (a = 4.147(1) Å, c = 6.711(2) Å, c/a = 1.618(1)), [145] (a = 4.149(1) Å, c = 6.715(1) Å, c/a = 1.6185(4)) and [146] (a = 4.1475 Å, c = 6.71 Å, c/a = 1.61784).

The values of the isotropic thermal shifts of the Mn and Te ions obtained by Rietveld refinement are 0.581(26) Å<sup>2</sup> and 0.421(10) Å<sup>2</sup>, respectively. These values are close to those obtained by neutron powder diffraction measurements (0.84(1) Å<sup>2</sup> for Mn and 0.57(1) Å<sup>2</sup> for Te) reported in [147]. At the time of publication, I did not find the corresponding values determined by X-ray powder diffraction in the literature, so it can be assumed that the mentioned parameters were determined for the first time by the XRD method.



Figure 8: An example of Rietveld method refinement for MnTe measured at temperatures of 313 K (a) and 623 K (b) [H3]. Experimental points are marked with red dots, and calculated curves are marked with a black solid line. The short vertical bars indicate the positions of the Bragg reflections, for the temperature of 623 K the second set of dashes corresponds to the MnTe<sub>2</sub> phase. The lower blue lines show the difference between the experimental and calculated points.

With increasing temperature, the values of both the  $\alpha$ -MnTe lattice parameters and their c/a ratio increase smoothly over the entire temperature range studied (Figure 9). Compared to previous hightemperature studies [148-151] (data from these works are included in the graphs in Figure 9 for comparison), the present results cover a wider temperature range, have a larger number of measured temperature points, and show a clear trend in the change of the network parameters. The obtained temperature curves show a change in the slope of the a(T) and c(T) relationship at about 308 K (Néel temperature  $(T_N)$ ) due to the magnetic phase transition occurring at this temperature [11]. The increase in the c/a ratio with temperature indicates the occurrence of thermal expansion anisotropy in the c direction for  $\alpha$ -MnTe, with the nature of the anisotropy being similar for temperatures higher and lower then  $T_N$ . By approximating the obtained relationships at temperatures above  $T_N$  with a linear function, I determined the average values of the thermal expansion coefficient (TEC), which are  $\alpha_a =$  $1.62 \times 10^{-5} \text{ K}^{-1}$  and  $\alpha_c = 2.86 \times 10^{-5} \text{ K}^{-1}$ . These values for the lattice parameters a and c are 10% and 20% higher and 30% and 20% lower, respectively, than the TEC values estimated from previous literature data (ref. [149] and ref. [150] respectively). Moreover, the TEC value for the  $\alpha$ -MnTe phase is almost an order of magnitude larger than that for  $\beta$ -MnTe (5×10<sup>-6</sup> K<sup>-1</sup>) [153].

In the high temperature range from 500 K to 1023 K, I observed a partial transformation of MnTe into a MnTe<sub>2</sub> phase with a pyrite structure (space group: *Pa*-3) (see Fig. 8b). From ref. [152] it appears that in the presence of an oxidizing atmosphere there is a transformation of 2  $\alpha$ -MnTe + 1/2O<sub>2</sub> $\rightarrow$ MnTe<sub>2</sub> + MnO starting at about 400 K and a transformation of MnTe<sub>2</sub> $\rightarrow$ MnTe + Te at about 990 K. Unfortunately, in the case of the present study, I could not detect the possible presence of a crystalline phase of MnO. The reason may be a size effect. In fact, small MnO precipitates do not contribute significantly to the diffraction signal intensities. It should be noted that all previous observations were not accompanied by a detailed quantitative analysis of the resulting phases. To remedy this situation, I have used the Rietveld method to determine the changes in the lattice parameter of the formed MnTe<sub>2</sub> compound with temperature and to determine its content relative to the  $\alpha$ -MnTe phase as a function of temperature. Both dependencies are shown in Figure 10. The content of the MnTe<sub>2</sub> phase gradually increases from its appearance in the diffraction patterns at 500 K to a level of 8-10% in the range from 600 to 1020 K. At temperatures around 1050 K, its content drops to about 0.5%, which, according to ref. [152], is due to the transformation of MnTe<sub>2</sub> $\rightarrow$ MnTe + Te. At temperatures above 1050 K, the MnTe<sub>2</sub> phase is no longer present.





Figure 9: Temperature dependence of  $\alpha$ -MnTe lattice parameter values a (a), c (b) and their ratio c/a (c) [H3]. Black squares in the wide temperature range represent current experimental data. Literature data are marked with asterisks [148], open triangles [151], open squares [149], and open circles [150].



Figure 10: Temperature dependence of the  $MnTe_2$  lattice parameter (a) and the the  $MnTe_2$  phase content (b) observed in the high temperature range [H3].

# Structure of selected $RM_3(BO_3)_4$ compounds doped with transition metal and rare earth ions and their elastic properties under high temperature conditions.

 $RM_3(BO_3)_4$ , crystals with a huntite structure, where *R* is rare earth or yttrium ions and *M* is Al, Fe, Ga, Sc or Cr, have recently been actively studied for various physical properties and applications, as mentioned in the introduction. Although a large part of these materials had already been synthesized and described in the literature [154 the full structure was given only for a few compounds (YAl<sub>3</sub>(BO<sub>3</sub>)<sub>4</sub> [155,156] NdGa<sub>3</sub>(BO<sub>3</sub>)<sub>4</sub> [157]) and the structural behavior of these materials under high temperature conditions was almost unknown. Therefore, while carrying out the structural characterization for magnetic and optical studies of crystals based on YGa<sub>3</sub>(BO<sub>3</sub>)<sub>4</sub>, EuGa<sub>3</sub>(BO<sub>3</sub>)<sub>4</sub>, YAl<sub>3</sub>(BO<sub>3</sub>)<sub>4</sub>, EuAl<sub>3</sub>(BO<sub>3</sub>)<sub>4</sub> and TmAl<sub>3</sub>(BO<sub>3</sub>)<sub>4</sub> compounds, I decided not to limit myself to just refining the structure of these materials under study, but to fill in the lack of knowledge regarding the behavior of these materials at high temperature conditions.

The elementary cell of borate crystals  $RM_3(BO_3)_4$  in the structure of  $CaMg_3(BO_3)_4$  huntite with space group R32 [155,156,157] contains Z = 3 formal units. The elementary cell of the compound consists of trigonal prisms, octahedra and triangles formed by oxygen ions with  $R^{3+}$ ,  $M^{3+}$  and  $B^{2+}$  ions in the center, respectively. Rare earth ions are distributed along the *C* axis in slightly distorted prisms formed by oxygen ions, in which the upper and lower triangles are slightly rotated with respect to each other. The  $M^{3+}$  ions are located inside the oxygen octahedra, which, coupled by their edges, form twisted columns elongated in the direction of the *C* axis. Boron atoms occupy two unequal positions, B(1) and B(2), inside oxygen triangles of two types: B(1) ions are located in triangles perpendicular to the triple axis, separated by *R* prisms, while B(2) ions are triangles connecting twisted columns of oxygen octahedra containing metal ions. A graphical model of such a structure is shown in Figure 11. The positions of the atoms in the crystal according to the representation of the elementary cell in the hexagonal axes can be shown as follows:

R	3а	(0,	0, 0);
М	9d	( <i>x</i> ,	0, 0);
B(1)	3b	(0,	0, ½);
B(2)	9e	( <i>x</i> ,	0, ½);
O(1)	9e	( <i>x</i> ,	0, ½);
O(2)	9e	( <i>x</i> ,	0, ½);
O(3)	18f	( <i>x</i> ,	y, z).

TmAl<sub>3</sub>(BO<sub>3</sub>)<sub>4</sub> crystal doped with 0.1% Cr<sup>3+</sup> [H5] ions, two YAl<sub>3</sub>(BO<sub>3</sub>)<sub>4</sub> crystals doped with 0.1% Cr<sup>3+</sup> [H5] and 0.1% Co<sup>3+</sup> [H4] and two EuAl<sub>3</sub>(BO<sub>3</sub>)<sub>4</sub> crystals doped with 0.2% Tb<sup>3+</sup> [H7], 0.2% Cr<sup>3+</sup> [H5] and 0. 2% Co<sup>3+</sup> [H4] as well as three YGa<sub>3</sub>(BO<sub>3</sub>)<sub>4</sub> crystals including one undoped [H6] and two doped with 0.2% Cr<sup>3+</sup> [H5] and 0.2% Er<sup>3+</sup> [H6] ions and one EuGa<sub>3</sub>(BO<sub>3</sub>)<sub>4</sub> crystal doped with 0.2% Tb<sup>3+</sup> [H7] were obtained from melt solution by spontaneous crystallization [154]. The crystals, which ranged in size from 0.5 to 3 mm, were transparent and had well-developed natural planes/surfaces.



Figure 11: Crystal structure of  $RM_3(BO_3)_4$  materials, where R is a rareearth element or ito yttrium, M stands for trivalent ions  $Al^{3+}$ ,  $Ga^{3+}$ ,  $Fe^{3+}$ ,  $Sc^{3+}$ ,  $Cr^{3+}$ , with space group R32h.

I performed X-ray structural and thermostructural studies of these materials using a laboratory diffractometer (X'Pert Pro Alpha1 MPD, Panalytical). For measurements under normal conditions, the diffractometer was equipped with a Ge (111) primary beam monochromator and a position sensitive linear semiconductor detector (X'Celerator) [158]. Measurements at high temperatures (300-1073 K) were performed using an Anton Paar high-temperature furnace chamber (model HTK 1200 N) equipped with a capillary extension sample holder.  $Cu_{K\alpha}$  radiation was used as the source beam. The crystals were studied in powder form. The data obtained, in the form of X-ray diffractograms for individual temperatures, were analyzed using the Rietveld method to refine the structural parameters. In order to calculate the thermal expansion coefficients, the obtained relations l(T) were first fitted with a Laurent polynomial:  $l(T) = C_0 + C_1 \cdot T + C_{-1}/T$ , (where l is a, c or V) and then the thermal expansion coefficients were size of  $\alpha_l(T) = (dl/dT)/l(T)$ .



Figure 12. Graphical results of structure refinement of  $EuAI_3(BO_3)_4$  doped with 0.2%  $Cr^{3+}$  (a) and  $YGa_3(BO_3)_4$  doped with 0.2%  $Er^{3+}$  ions (b) by the Rietveld method. Red open dots - experimental data, black solid line - fitted diffraction model, vertical green bars - Bragg peak positions (the second set of bars corresponds to the  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> phase), solid blue line - difference between experimental data and model.

Position	хM	<i>x</i> B(2)	<i>x</i> O(1)	xO(2)	xO(3)	<i>y</i> O(3)	zO(3)	Lattice	Ref.
								parameters	
Material								a, c , Å	
TmAl <sub>3</sub> (BO <sub>3</sub> ) <sub>4</sub> :	0.5569(3)	0.449(1)	0.8554(5)	0.5836(8)	0.4396(5)	0.1347(5)	0.5259(6)	9.27050(5)	[H5]
0.1% Cr								7.21351(6)	
YAI3(BO3)4:	0.5547(3)	0.4475(8)	0.8599(5)	0.5843(6)	0.4469(4)	0.1507(4)	0.5221(5)	9.28103(5)	[H4]
0.1% Co								7.22793(5)	
YAI <sub>3</sub> (BO <sub>3</sub> ) <sub>4</sub> :	0.5563(2)	0.4477(6)	0.8529(3)	0.5862(4)	0.4469(3)	0.1429(3)	0.5265(6)	9.28224(6)	[H5]
0.1% Cr	0.550440	0.440(0)	0.074/1	0.550(4)	0.440(4)	a (=a(i)	0 -0-(4)	7.23057(6)	
EuAl <sub>3</sub> (BO <sub>3</sub> ) <sub>4</sub> :	0.5521(4)	0.410(3)	0.874(1)	0.558(1)	0.440(1)	0.153(1)	0.535(1)	9.30924(9)	[H4]
0.2% 00	0.5554(4)	0.447/4	0.0540(0)	0.5040(0)	0.4404(0)	0 4 4 4 5 / 5	0 5000/7)	7.27097(9)	61.151
EUAI3(BO3)4:	0.5554(4)	0.447(1	0.8546(6)	0.5849(9)	0.4424(6)	0.1415(5	0.5300(7)	9.31172(8)	[H5]
	0 5551(7)	0.446(2)	0.9644(6)	0.570(1)	0.4456(6)	0.1264/6)	0 5004/0)	0.2020(1)	[1]7]
0.2% Th	0.5551(7)	0.440(2)	0.0044(0)	0.579(1)	0.4450(0)	0.1304(0)	0.5224(6)	9.3069(1) 7.2686(1)	[[[]]]
0.2 /0 10								7.2000(1)	
YGa3(BO3)4:	0.5508(1)	0.4438(9)	0.8630(6)	0.5837(5)	0.4514(5)	0.1435(4)	0.5070(5)	9.4487(1)	[H6]
	0.0000(1)	011100(0)	0.0000(0)	0.0001 (0)	••••••••(•)	••••••(1)	0.001.0(0)	7.4477(1)	[]
YGa <sub>3</sub> (BO <sub>3</sub> ) <sub>4</sub> :	0.5505(1)	0.449(1)	0.8638(6)	0.5861(6)	0.4497(6)	0.1420(5)	0.5088(7)	9.44905(9)	[H5]
0.1% Cr								7.4546(1)	
YGa <sub>3</sub> (BO <sub>3</sub> ) <sub>4</sub> :	0.5513(1)	0.443(1)	0.8640(6)	0.5877(6)	0.4517(6)	0.1442(5)	0.5074(6)	9.4520(1)	[H6]
0.2% Er								7.4513(1)	
EuGa <sub>3</sub> (BO <sub>3</sub> ) <sub>4</sub> :	0.5515(1)	0.452(1)	0.8673(6)	0.5813(6)	0.4548(5)	0.1372(5)	0.5156(7)	9.4716(1)	[H7]
0.2% Tb								7.4773(1)	
YAI3(BO3)4	0.5554(2)	0.4436(6)	0.8512(5)	0.5907(5)	0.4499(4)	0.1498(4)	0.4786(4)	9.295(3)	[155]
	0.550.440	<b>0</b> 111(1)	0.0700(0)	0.50440	0.4505(0)	0.4.40=(0)	0 = ( 0 0 ( 0 )	7.243(2)	
NdGa <sub>3</sub> (BO <sub>3</sub> ) <sub>4</sub>	0.5524(1)	0.444(1)	0.8539(8)	0.591(1)	0.4507(8)	0.1467(8)	0.5192(8)	9.500(6)	[157]
								1.502(2)	

Table 1. Rietveld method-refined lattice parameters and free coordinates of atoms in  $RM_3(BO_3)_4$  crystals, without and with dopants of rare earth ions and metals.

For the phase and structural analysis of the investigated materials, X-ray diffraction measurements were performed under normal conditions. The tested materials were single phase, crystallized in the structure of Mg<sub>3</sub>Ca(CO<sub>3</sub>)<sub>4</sub> huntite with space group *R*32. However, it should be mentioned that in the case of gallium borates, single strand gallium oxide ( $\beta$ -Ga<sub>2</sub>O<sub>3</sub>) crystals were also crystallized from the melt solution as a side phase, the crystals of which could not always be separated from the gallium borate crystals, but the content of this phase did not exceed a few percent and did not significantly affect the analysis of the structure of the studied materials.

The structure analysis of the materials, performed by the Rietveld method, was based on input structure models previously published for the compounds YAl<sub>3</sub>(BO<sub>3</sub>)<sub>4</sub> [155] in the case of aluminum borates and NdGa<sub>3</sub>(BO<sub>3</sub>)<sub>4</sub> [157] in the case of gallium borates. A summary of the refined lattice parameters and atomic positions for all the samples studied is given in Table 1, which also includes the parameters of the crystal models published in the above-mentioned references [155] and [157] for the crystals YAl<sub>3</sub>(BO<sub>3</sub>)<sub>4</sub> and NdGa<sub>3</sub>(BO<sub>3</sub>)<sub>4</sub>, respectively. Data on the structure of borates based on YGa<sub>3</sub>(BO<sub>3</sub>)<sub>4</sub> and EuGa<sub>3</sub>(BO<sub>3</sub>)<sub>4</sub> are, to the author's knowledge, published for the first time in the work underlying this dissertation, although the lattice parameters of these materials were published earlier [154] with less precision. As can be seen, the exchange of the rare earth type in these compounds leads to an increase in the elemental cell size proportional to the increase in the size of the substituted ion. This effect also occurs when metal ions are exchanged from  $Al^{3+}$  to  $Ga^{3+}$ , as shown in Figure 13a. where the elemental cell volume of aluminum borates and gallium borates is plotted as a function of the size of the rare earth ion contained in the matrix crystal lattice. In addition, the substitution of larger ions leads to an elongation of the elementary cell along the *c*-axis, as indicated by an increase in the value of the c/a ratio (see Figure 13b). The observed relationships are consistent with literature data and the results of my previous work. The literature values in Figures 13a and 13b are taken from the following sources: Ref. [159,154,160] for TmAl<sub>3</sub>(BO<sub>3</sub>)<sub>4</sub>, matrix compounds ref. [155,154,156] for YAl<sub>3</sub>(BO<sub>3</sub>)<sub>4</sub>, ref. [161,162] for HoAl<sub>3</sub>(BO<sub>3</sub>)<sub>4</sub>, ref. [154,163] for EuAl<sub>3</sub>(BO<sub>3</sub>)<sub>4</sub> ref. [154,164] for NbAl<sub>3</sub>(BO<sub>3</sub>)<sub>4</sub>, ref. [154] for YGa<sub>3</sub>(BO<sub>3</sub>)<sub>4</sub>, ref. [165] for HoGa<sub>3</sub>(BO<sub>3</sub>)<sub>4</sub> and ref. [157] for NdGa<sub>3</sub>(BO<sub>3</sub>)<sub>4</sub>. Doping the crystals with metal or rare earth ions in the parts per thousand range does not significantly affect the changes in lattice parameters or atomic positions. The small differences we observe between the structural parameters for similar compounds can rather be attributed to the imperfections of the crystals studied. In the same way, no clear correlations have been observed in the changes in atomic positions with the change in ion type in  $RM_3(BO_3)_4$ , crystals, it can be said that the differences in atomic positions are not significant.



Rysunek 13. Volume (a) and c/a ratio (b) of borates with huntite-type structure as a function of the size of the rare earth ion. Experimental data [H4 - H7], are marked with solid rectangles, literature data with empty spheres. Dashed lines - "guide to the eye".

Investigation of these materials under high temperature conditions showed that they are phase and structurally stable over the entire temperature range from 302 to 1083 K. With increasing temperature, no additional peaks appeared on the diffractograms indicating a phase transition or decomposition of the material into other phases. The lattice parameters and elementary cell volumes increase smoothly with increasing temperature (see Fig. 14). An increase in the c/a ratio with increasing temperature is observed, indicating a strong anisotropy in the thermal expansion of the material, but the slopes of these curves are different for aluminum-based borates compared to gallium-based borates. Thus, analysis of the relative changes in lattice parameters with temperature shows that for aluminum borates the lattice parameter c increases with temperature about 2.5 times faster than the lattice parameter a, while for gallium borates it is about 3.5 times faster.

This result shows an increase in thermal expansion anisotropy for Ga-based borates compared to the observed anisotropy for Al-based borates. The difference in the average values of the expansion coefficients for the lattice parameters *a* and *c* over the investigated temperature range also confirms the expansion anisotropy. For example,  $\alpha_a$  and  $\alpha_c$  for EuAl<sub>3</sub>(BO<sub>3</sub>)<sub>4</sub>:Tb are 3.8 MK<sup>-1</sup> and 12.1 MK<sup>-1</sup>, respectively. The exchange of the metal ion results in a small decrease of  $\alpha_a$  and an increase of  $\alpha_c$  for EuGa<sub>3</sub>(BO<sub>3</sub>)<sub>4</sub>:Tb – 3.1 MK<sup>-1</sup> and 13.5 MK<sup>-1</sup>, respectively. The values are almost the same when the rare earth ion is exchanged and are for  $\alpha_a$  and  $\alpha_c$  3.7 MK<sup>-1</sup> and 12.0 MK<sup>-1</sup> as well as 3.1 MK<sup>-1</sup> and 13.4 MK<sup>-1</sup> respectively for YAl<sub>3</sub>(BO<sub>3</sub>)<sub>4</sub> and YGa<sub>3</sub>(BO<sub>3</sub>)<sub>4</sub> doped with chromium, in addition for TmAl<sub>3</sub>(BO<sub>3</sub>)<sub>4</sub>:Cr the values are 3.47 MK<sup>-1</sup> and 12.0 MK<sup>-1</sup> for  $\alpha_a$  and  $\alpha_c$  respectively.



elemental cell volume V(1) (d). Legend shown on HoGa<sub>3</sub>(BO<sub>3</sub>)<sub>4</sub> - literature data from ref. [165].

 $MK^{-1}$ .



YGa<sub>3</sub>(BO<sub>3</sub>)<sub>4</sub> - ref. [H6]

EuAl<sub>3</sub>(BO<sub>3</sub>)<sub>4</sub>: 0.2% Cr - ref. [H5]

EuAl<sub>3</sub>(BO<sub>3</sub>)<sub>4</sub>: 0.2% Co - ref. [H4] EuAl<sub>3</sub>(BO<sub>3</sub>)<sub>4</sub>: 0.2% Tb - ref. [H7] YAl<sub>3</sub>(BO<sub>3</sub>)<sub>4</sub>: 0.1% Cr - ref. [H5]

YAI<sub>3</sub>(BO<sub>3</sub>)<sub>4</sub>: 0.1% Co - ref. [H4]

At the time of publication of most of the results presented in this dissertation, no other work was available for comparison, but as of today it can be said that the results obtained are comparable to those for HoGa<sub>3</sub>(BO<sub>3</sub>)<sub>4</sub> [165] published by another group in January 2020. In that paper, a volumetric thermal expansion coefficient of 13.4 MK<sup>-1</sup> is reported for the temperature range from 403 to 503 K, while for the present results the  $\alpha_V$  coefficient for gallium yttrium borates (which are close to the size of rare earth ions) is 17.7 MK<sup>-1</sup>. This difference is probably due to the small number of experimental points and the limited range of temperatures studied in the aforementioned publication.



Figure 15: Temperature variation of volumetric coefficient of thermal expansion of aluminum and gallium borates.

#### Summary

1 I have carried out diffraction studies from which I have obtained detailed quantitative information on the thermostructural and elastic properties of (Pb,Cd)Te salt-type crystals. These data were not previously available for the (Pb,Cd)Te system, a PbTe-based thermoelectric material. The results show how the partial replacement of Pb ions by Cd ions in the PbTe lattice affects the temperature stability of the material, the lattice parameter and its behaviour over a wide temperature range. I obtained unique information on the thermal expansion coefficient, atomic displacements and other thermostructural properties, such as compressibility, Debye temperature or Grüneisen parameter. In particular, I showed that:

- the crystal lattice of the mixed crystal of (Pb,Cd)Te is less rigid than that of PbTe,

- the thermal expansion of the compound (Pb,Cd)Te is clearly greater than that of PbTe,

- the range of stability of the material at temperatures above room temperature is small,

- at higher temperatures, I discovered a unique behaviour of the PbTe-CdTe metastable solid solution, with a temperature-induced exit of Cd ions from the cationic positions in the PbTe matrix into the crystal volume (in the range T=500-900 K), followed by the return of cadmium to the cationic sub-

network of the PbTe matrix (for T>900 K), with a temperature-dependent behaviour of the lattice parameter similar to that of the matrix.

A fundamental increase in knowledge of the thermostructural properties of the PbTe-CdTe material system is important for further work on the application of lead telluride with functional Cd substituents in thermoelectric modules.

2 Using modern diffraction test methods using synchrotron radiation, more accurate , compared to previous experimental work, for the  $\alpha$ -MnTe compound (a magnetic semiconductor exhibiting alltermagnetism):

- I determined the temperature evolution of the lattice parameters a and c over a wide temperature range from 289 K to 1200 K,

- I determined the exact behaviour of the lattice parameters in the vicinity of Neel's temperature,

- I determined the average values of the linear thermal expansion coefficients over the investigated temperature range,

- I demonstrated the anisotropy of  $\alpha$ -MnTe thermal expansion in the c-direction, which occurs both below and above  $T_N$ ,

- I confirmed and quantitatively analyzed the partial decomposition of the  $\alpha$ -MnTe phase to the MnTe<sub>2</sub> phase with a pyrite-type structure at about 500 K and the reverse process at about 1050 K.

3. I have refined the structure parameters of aluminium and gallium borates doped with metal and rare earth ions - materials relevant to laser sources. For the first time I showed the structure of compounds:

 $\begin{array}{l} -EuAl_{3}(BO_{3})_{4},\\ -TmAl_{3}(BO_{3})_{4},\\ -YGa_{3}(BO_{3})_{4},\\ -EuGa_{3}(BO_{3})_{4}.\end{array}$ 

I was the first to perform thermal expansion studies of aluminum and gallium borates under high temperature conditions. In these studies:

- I showed that the volumetric thermal expansion marginally depends on the type of rare earth ion and metal ion placed in the borate matrix with a huntite-type structure,

- I showed the anisotropic nature of the thermal expansion of these materials,

- I showed that the anisotropy of gallium borates is greater than that of aluminum borates.

#### Other important scientific achievements

#### Structural properties of superconducting (La,Sr)CuO<sub>4</sub> with Ni

I have shown the structural evolution of the compound  $La_{1.85}Sr_{0.15}Cu_{1-x}Ni_xO_4$  ( $0 \le x \le 0.19$ ) with  $K_2NiF_4$  (S.G. *14/mmm*) structure as a function of nickel ion content [166], which governs the superconducting properties in this material (disappearing at Ni concentrations around 5%). Previous studies on the LSCO structure of doped Ni showed the evolution of the lattice parameters of a given material for only a few x-values and exhibited a significant scattering of values. Using X-ray powder diffraction, I determined the structure of this material for more than 15 compositions with nickel content from 0 to 16%. I showed an almost linear behavior of variation for the lattice parameters *a* and *c* of this material, their ratio (*c/a*) and volume and also calculated the coefficients of these relationships for all the mentioned parameters. I showed that the atomic coordinate  $z_{O(2)}$  is constant, and  $z_{La/Sr}$ 

increases with increasing nickel content. Also, I showed that an increase in Ni concentration in the elemental cell causes a shrinkage in the volume of (Cu/Ni)O6 octahedra with an increase in the (Cu/Ni)-O(1) distance and a decrease in the (Cu/Ni)-O(2) distance.

### **Elastic properties of rare earth vanadates**

I have also been engaged in the study of the elastic properties of rare earth vanadates with a zirconium-type structure (RVO<sub>4</sub>, where R = Sc, Y, La-Lu), which show interesting physical properties in terms of their practical application. As part of this scientific activity, I have obtained a series of new quantitative information on the behavior of the terbium orthovanadate elemental cell under high pressure [167]. Using *in situ* energy dispersive X-ray diffraction, I showed the evolution of the TbVO<sub>4</sub> elemental cell in the pressure range up to 7.28 GPa. On the basis of the obtained results, for the first time relying on diffraction data, I determined the dependence of lattice parameters and their ratio on the Birch-Murnaghan type equation of state of the material under study and determined the value of the bulk compressibility modulus and its pressure derivative. As part of this activity, I have also actively participated in work on the behavior of other such compounds under high pressures, such as dysprosium orthovanadate [168,169] and lanthanum orthovanadate [170].

# 4. Information on scientific activity in national and international institutions

My scientific career started during my studies at the Faculty of Physics of the **Donetsk National University** (Ukraine). The scope of my scientific work was to obtain polycrystalline fullerene layers on titanium substrates by thermal deposition methods and to determine the structure and corrosion resistance of these layers depending on their thickness and the conditions of deposition and post-deposition annealing in an argon atmosphere. The results of these studies formed the basis of my master's thesis under the supervision of **Ph.D. Antonina Trotsan**. Some of the results described in the thesis were published in the journal "Izvestiya Akademii Nauk, seriya fizicheskaya" [171] in 2002.

After receiving my Master's degree, I did my Ph.D. studies at the **Institute of Physics of the Polish Academy of Sciences** in the Laboratory of X-ray and Electron Microscopy Research in the Group of applied crystallography (SL1.3) under the supervision of **Professor Dr. hab. Wojciech Paszkowicz**. I performed studies on the structural properties as a function of temperature and pressure of gallium nitride, aluminum nitride [172,173], indium nitride, silicon nitride [174] and germanium nitride, as well as diamond [174] and gold [176] the last two materials can serve as an internal standard in thermostryctural studies and increase the accuracy of the results obtained. Most of these studies were performed using synchrotron radiation in cooperation with foreign centers in Germany (**DESY**), and Denmark (**Technical University of Denmark**). In addition, I performed numerous diffraction studies to characterize the structure of oxide materials such as ZnO and ZnMnO thin films [177-182] and YBa<sub>2</sub>Cu<sub>3</sub>O<sub>7</sub> / La<sub>1-x</sub>Sr<sub>x</sub>MnO<sub>3</sub> multilayers [183-185]; metallic and semiconductor thin films: W-Ti-N [186,187], Ta-Si-N [188], Fe [189], Cr/Gd multilayers [190]; Zn<sub>1-x</sub>Mg<sub>x</sub>Se and Zn<sub>1-x-y</sub>Mg<sub>x</sub>Be<sub>y</sub>Se crystals [191] within the framework of cooperation with other divisions of the **IF PAN**, the **Lukasiewicz - Institute of Microelectronics and Photonics** in Warsaw and the **Nicolaus Copernicus University** in Torun.

After receiving my Ph.D., I continued my scientific work in the Applied Radiography Group (SL1.3) headed by **Prof. Dr. hab. Wojciech Paszkowicz**.

My immediate scientific interest became structural studies of materials at high and low temperatures and high pressures.

As part of the scientific projects provided by our team at the synchrotron beamlines in Hamburg (**DESY, Hasylab**), I was involved in the determination of the equation of state of the polymorphs DyVO<sub>4</sub> [168,169] and TbVO<sub>4</sub> with zirconium structure [167], the determination of the effect of pressure on the structural and magnetic properties  $La_{1-x}Sr_xCoO_{3-9}$  [192], determination of the compressibility of  $SrSi_2O_2N_2$  compounds doped with europium ions [194,195] and CaMnO<sub>3</sub> [196], determination of the thermal expansion of CuInSe<sub>2</sub> over a wide temperature range [193,197], determination of the thermostructural and elastic properties of Pb<sub>1-x</sub>Cd<sub>x</sub>Te in low temperature and high pressure conditions [H1] and at high temperature [H2]. The latter two papers were carried out in collaboration with **Prof. Dr. hab. Wojciech Szuszkiewicz**. Also with the support of **Prof. Szuszkiewicz**, high-temperature structural studies of manganese telluride with NiAs-type structure were performed [H3].

In addition, several projects were carried out by our team at the University of Lund (Sweden) at the **MAX III** synchrotron, where we performed pressure studies to determine the equation of states of silver behenate [198] and lanthanum orthovanadate with a monazite-type structure [170]. I also participated in pressure [198] and high temperature [199] studies of  $Ca_9RV_7O_{28}$  (R = La, Nd, Gd) compounds at the **ALBA** (Spain) and **ESRF** (France) synchrotrons, and in ultrafast structure change studies of metals and their alloys [201] and overcooled liquid metals at the **DESY** (Germany) and with free-electron lasers at the **XFEL** (Germany) and **SwissFEL** (Switzerland).

I also did a research internship as part of the CEICERES scholarship programme, Sincrotrone Trieste (Elettra), where I was involved in the construction of an X-ray lab and studied ZnO-based nanocrystals.

In addition, I collaborate with more than 16 scientific departments and environmental laboratories of IFPAN. For them, I have performed numerous analyses of the structure of various types of polycrystalline, nanocrystalline materials and thin films by powder X-ray diffraction and reflectometry methods.

The most fruitful collaboration was:

- with the scientific department headed by **Prof. Dr. hab. Tomasz Story**, where I performed characterization of the structure of epitaxial thin films of Pb<sub>1-x</sub>Sn<sub>x</sub>Se [202], (Ge, Mn, Sn)Te [203], ferromagnetic semiconductor layers Ge<sub>1-x</sub>Mn<sub>x</sub>Te/PbTe//KCl [204], Sn<sub>1-x</sub>Mn<sub>x</sub>Te crystals [205] and PbTe-CdTe system [206]. I also participated in the research project "Development of a technology for the manufacture of a new type of thermoelectric modules for the conversion of low-parameter waste heat into electricity", in which I performed the characterization of materials by X-ray diffraction methods.

- with **Prof. Dr. hub. Wojciech Szuszkiewicz**, in addition to the above mentioned work, I performed studies of phonon scattering in solid solutions of (Pb,Cd)Te by inelastic X-ray scattering [207] and structural characterization of (Pb,Cd)Te crystals [208-212] and (Hg,Cd)Te thin films [213], for which there was a study of anisotropy of mechanical properties.

- with the Scientific Department headed by **Dr. hab. Anna Niedźwiecka**, I studied the structural and phase properties of light-converting single-component and core-shell nanoparticles based on NaYF<sub>4</sub> [214-217] and Gd<sub>2</sub>O<sub>3</sub> [218-221] compounds doped with rare earth and transition metal ions, as well as  $ZnAl_2O_4$ :( $Er^{3+}$ , Yb<sup>3+</sup>) [222], Fe<sub>2</sub>O<sub>3</sub>:(Y) [223] and Y<sub>3-0.02-x</sub>Er<sub>0.02</sub>Yb<sub>x</sub>Al<sub>5</sub>O<sub>12</sub> [224].

In 2012, I established a collaboration with the **Institute of Physics of the Czech Academy of Sciences** (Prague), Department of Analysis of Functional Materials, headed by **Ing. Ph.D. Jan Lancok**, and in particular directly with **Ph.D. Andriy Prokhorov**. We are united by our interest in the physical properties of so far poorly studied multicomponent systems of aluminum and gallium borates with rare-earth elements are  $RM_3(BO_3)_4$ , where *R* is rare-earth or Y ions and *M* is Al or Ga ions. In the course of this collaboration, I was involved in the study of the structure of these materials and their behavior under high temperature conditions (thermal stability, thermal expansion, expansion anisotropy) [159,163,H4,H5,225,H6,226,H7]. Most of the results of these studies became the basis of the present habilitation work.

Since 2015, I have maintained a collaboration with the **Institute of Nuclear Problems** (Otwock-Swierk, Poland), with a team led by **Dr. hab Katarzyna Nowakowska-Langer**, for whom he performs structural studies of thin films synthesised by pulsed magnetron sputtering with variable frequency plasma generation. These are mainly copper nitride thin films [227-230], aluminium nitride thin films [231] and molybdenum nitride [232]. I have also analysed the structure and morphology of metallic thin films: molybdenum [233] and tungsten [234], Fe-Cu [236] and Ni [238] alloys. I also used X-ray diffraction methods to characterise TiO<sub>2</sub> thin films obtained by pulsed magnetron sputtering with different concentrations of reaction atmosphere and sputtering modes [236,237].

Also in the last three years, a collaboration has been established with the **Taras Shevchenko National University in Kiev, Ukraine.** Together with **Dr.S. Serhiy Nedilko's** group, a project funded by the National Agency for Academic Exchange (NAWA) was carried out under the title "Research of vanadate nanoparticles for extraction of light from ultraviolet radiation". The objects of research were selected orthovanadate nanoparticles isovalent and heterovalent doped with the formula  $La_{1-x-y}Er_{x/2}Eu_{x/2}Ca_yVO_4$  ( $0 \le x \le 0.3$ ,  $0 \le y \le 0.2$ ),  $EuVO_4$ :xCa ( $0 \le x \le 0.2$ ) i  $La_{1-x}Sm_xVO_4$ :Ca ( $0.05 \le x \le 0.2$ ). The tangible results of this collaboration are two journal articles [239-241].

# **5.** Information about the achievements in teaching, organization and popularizing science or art

#### **Didactic achievements**

I was the associate supervisor of PhD student Houri S. Rahimi Mosafer (she has defended the thesis in December 2023).

I was the supervisor of the intern Mateusz Modzelewski student of the Faculty of Physics of the Warsaw University of Technology in the period from 01.07.2024 to 12.07.2024

I was the supervisor of the participant in the "ZDOLNI" programme of the National Children's Fund, trainee Kornelia Gościmińska, from 16.09.2024 to 27.09.2024.

I was one of the tutors of a physics workshop for talented young people. The workshop was organized in cooperation with the National Children's Fund in Institute of Physics of the Polish Academy of Sciences, 20.01-25.01.2014 and 29.01-02.02.2024.

As part of the environmental laboratory activity, jointly with Prof. Dr. hub. W. Paszkowicz I supervised interns, fourth-year students from the Warsaw University of Technology in 2016-2018.

Individual tuition for intern Olga Trubayeva in laboratory SL1.3 on experimental methods used in our laboratory.

In 2002 I was a lecturer of physics at the Building Technical School (Makeevka, Ukraine)

# **Organisational achievements**

In frame of scientific activity of the SL1.3 laboratory I led a research project entitled "High-pressure diffraction study of selected zircon-type and scheelite-type rare-earth orthovanadates", carried out at Hasylab in Hamburg, Germany in January and October 2012.

Also I led the team research project 'In-situ high temperature microstructure evolution of (Ga,Mn)As' carried out at ELETTRA in Trieste, Italy in February 2016.

In 2019, in frame of bilateral exchange of scientists between Poland and Ukraine (NAWA) and led the international research project 'Research of vanadate nanoparticles for light extraction from ultraviolet radiation', in collaboration with Taras Shevchenko National University of Kyiv. (The project was completed in December 2021)

# Achievements in the popularisation of science

In 2015, 2018 and 2023, I participated in the open day of the Institute of Physics of the Polish Academy of Sciences, where I presented the laboratory of applied crystallography, gave demonstrations of the use of X-ray diffraction for structure and phase analysis of materials.

# 6. Other information - development of measurement instruments and methods

# The development of the measuring facility

During my stay in Italy as part of the CERES scholarship program, I was engaged in the design and construction of the Hard X-ray laboratory, with a particular focus on the construction of the crystallographic research station.

At the Institute of Physics of the Polish Academy of Sciences, in the Laboratory of X-ray and Electron Microscopy Research in the Group of Applied Crystallography (SL1.3), as part of the implementation of the grant of Prof. dr hab. Wojciech Paszkowicz, I designed, participated in the installation and developed research procedures for high-temperature in-situ powder diffraction research techniques.

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