1. PHD PROJECT DESCRIPTION (4000 characters max., including the aims and work plan)

Project title: *Positron annihilation lifetime spectroscopy in mixed crystals*

1.1 Project goals

- Modifications of positron annihilation lifetime spectrometer (PALS) available at Center of Quantum Optics, Nicolaus Copernicus University in Torun, to carry out the characterization of positron lifetimes in mixed crystals (alloys) as a function of the temperature. Careful calibration of the experimental system in a new configuration.
- Characterization of positron lifetimes in chosen mixed crystals (binary and ternary alloys). Analysis of acquired data using available theories for positron interaction with condensed matter. The identification of defects, particularly a careful study of shallow positron traps and charge states of vacancies. The search for correlation between defects and the crystal fabrication method, the post-fabrication treatment of the sample, and the alloy content.

1.2 Outline

Mixed crystals are the multicomponent systems of II-VI and III-V semiconductor compounds. The great attention devoted to this class of materials is triggered by their potential applications of industrial significance, such as nuclear radiation detectors, electro-optic modulators, and photorefractive devices [1]. Their superior optical, electrical, and thermal properties over other competitive materials make them good candidates for some commercial devices. Moreover, they are characterized by great flexibility in engineering these properties. The careful choice of crystal composition gives excellent control over these materials' electrical, optical, and thermal properties. However, despite great research efforts, devices based on semiconductive mixed crystals are hardly ever produced due to the technical difficulties and related high costs in fabricating high-quality crystals. The main limiting factor is the large number of defects formed during the growth of the multicomponent crystal. The problem is quite complex since each particular method for bulk crystal growth – melt, solution, and vapor growth – introduces different compositions, densities, and distributions of defects. Another issue is identifying and removing extrinsic impurities introduced during the fabrication process [2], a typical problem associated with semiconductor manufacturing technology.

Moreover, the internal structures of multicomponent materials are known to be very sensitive to the post-fabrication treatment of crystals. Consequently, there still needs to be more knowledge about the relationship between the fabrication method, the processing, the structure, and the properties of semiconductive alloys. In particular, the influence of lattice disorder on the properties of these materials and the evolution of related defects with the composition of alloys still needs to be fully understood.

Positron annihilation lifetime spectroscopy (PALS) is a powerful and nondestructive characterization technique used to study the microstructural properties of matter. In particular, PALS can identify particular point defects [3, 4] because positron lifetime is very sensitive to the size and the charge state of open volume. Moreover, the temperature dependence of positron lifetimes may reveal impurities at concentration levels inaccessible to other defect characterization techniques. Consequently, the method gives an outstanding possibility to study the correlation between the defect structure and the fabrication method, the post-fabrication treatment of the crystal, its structure, and its physical properties.

In summary, the main goal of this project is a systematic study of defect structures in mixed crystals using positron lifetime spectroscopy. The Ph.D. student will do the main experimental work with the fast–fast coincidence ORTEC PALS system equipped with plastic scintillators (St. Gobain BC418) and RCA 8850 photomultipliers [5, 6, 7]. One of the main elements of the work will be an adaptation of this setup for the characterization of positron lifetimes as a function of sample temperature.

1.3 Work plan

- Introduction to basics of the positron annihilation lifetime spectroscopy.
- Introduction to the methodology of PALS data analysis in solid bodies. Methods for defect identification using positron annihilation data.
- Taking part in the design and alignment of a new configuration of the experimental setup for the characterization of positron lifetimes as a function of the temperature; and calibration of the system.
- Characterization of positron lifetimes in chosen mixed (binary and ternary) crystals, analysis of PALS data, identification defect and their correlation with (i) fabrication method, (ii) the post-fabrication treatment, (iii) the structure, and (iv) the properties of alloys.

1.4 Literature

1. R. Triboulet, P. Siffert, *CdTe and Related Compounds; Physics, Defects, Hetero- and Nano-structures, Crystal Growth*, Surfaces and Applications, Elsevier, Oxford, 2009
2. M. Stavola (Editor), R. K. Willardson (Series Editor), E. R. Weber (Series Editor), *Identification of Defects in Semiconductors*, 1st Edition, Vol. 51A of *Semiconductors and Semimetals*, Academic Press, San-Diego, 1998.
3. R. Krause-Rehberg, H. S. Leipner, *Positron Annihilation in Semiconductors: Defect studies*, 1st Edition, Vol. 27 of Springer Series in Solid-State Sciences, Springer-Verlag, Berlin, 1999.
4. F. Tuomisto, I. Makkonen, *Defect identification in semiconductors with positron annihilation: Experiment and theory*, Rev. Mod. Phys. 85 (2013) 1583–1631
5. A. Karbowski, J. D. Fidelus, G.P. Karwasz, *Testing Ortec Lifetime System*, Mater. Sci. Forum 666, 155 (2011)
6. A. Karbowski, K. Fedus, J. Patyk, Ł. Bujak, K. Służewski, G. Karwasz, *Photoluminescence and positron annihilation lifetime studies on pellets of ZnO nanocrystals* Nukleonika 58(1) (2013), 189-194
7. M. Gorgol, R. Zaleski, A. Kierys, D. Kamiński, K. Strzałkowski, K. Fedus, *Positron lifetime spectroscopy of defect structures in* $Cd_{(1-x)}Zn_xTe$ *mixed crystals grown by vertical Bridgman-Stockbarger method*, Acta Crystalographica B 77, 515 - 525 (2021)

1.5 Required initial knowledge and skills of the PhD candidate

The candidate will develop all necessary knowledge and skills during the realization of the project. However, basic knowledge in at least one of the following areas is expected:

- basics in computer programming (preferably C++, Matlab, LabView),
- basic knowledge of electronics, circuits, and mechanical design
- basic knowledge of atomic and condensed matter physics

1.6 Expected development of the PhD candidate's knowledge and skills:

The Ph.D. candidate will gain the knowledge about:

- Positron annihilation spectroscopy
- Principles of matter-antimatter interaction
- Methods for analyzing complex experimental data using sophisticated theoretical models