TECHNO-CLS Newsletter

Scientific and Technological Highlights from the First Two Years

The TECHNO-CLS project aims to pioneer the development of next-generation gamma-ray light sources based on the channelling of ultra-relativistic particles through linearly, bent, or periodically bent crystals. The project unites multiple scientific disciplines, from multiscale modelling and materials science, to beamline engineering and optical diagnostics, in pursuit of Crystal-based Light Sources (CLS) capable of operating at photon energies greater than 10^2 keV.

This newsletter provides a comprehensive summary of progress made during the first two years of the project.

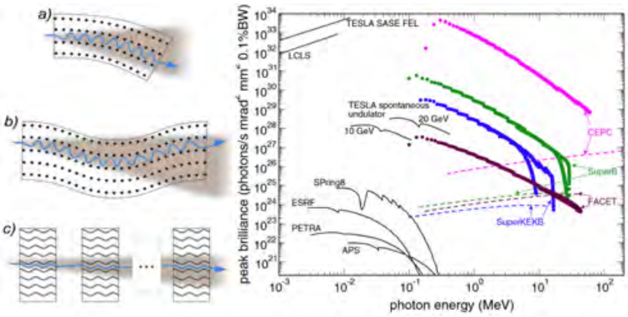

Figure 1: *Left*: Illustrations showing bent **(a)**, periodically bent **(b)**, and stacked **(c)** crystalline undulator crystals. *Right*: Plot showing the peak brilliances of radiation produced from carious light sources.

First Year Summary June 2022 - June 2023

Theory and Modelling

During the first year, efforts have focused on establishing the theoretical framework and computational protocols needed to design and analyse CLS devices.

The MBN Research Center has spearheaded efforts to simulate photon emission from periodically bent crystals using the MBN Explorer software. Studies included the characterisation of radiation emission in Small-Amplitude Short-Period (SASP) and Large-Amplitude Long-Period (LALP) crystal geometries, particularly for 10 GeV electrons and positrons. These simulations are crucial for defining feasible operational parameters for different CLS configurations. The results of these works can be found in Korol & Solov'yov, *Nucl. Instrum. Meth. B* **537**, 2023 and Sushko, *et al.* *Eur. Phys. J. D* **76**, 2022.

The MBN Research Center has also integrated radiative reaction forces into their molecular dynamics framework, MBN Explorer, enabling accurate simulation of energy loss effects for particles travelling within crystalline fields. They also developed a generic conceptual scheme for CLS device design, defining the key parameters required for reliable simulation of channelling radiation emission. This theoretical framework is detailed in Sushko *et al.* *Nucl. Instrum. Meth. B* **535**, 2023.

During the first year of the project, the Hellenic Mediterranean University focused on the numerical modelling of crystal structure deformation induced by acoustic wave excitation via piezoelectric transducers. Using finite element method simulations, they developed and analysed two technically favourable configurations for acoustically excited crystalline undulators: an Acousto-Optic Modulator-type scheme and a Vibrating Plate-type scheme. These models employed mechanical transient analysis to simulate the dynamic response of silicon, germanium, and diamond crystals under acoustic wave excitation at MHz frequencies, with the aim of defining viable operational parameters for dynamic periodic bending suitable for CLS applications.

In addition to mechanical simulations, the Hellenic Mediterranean University also performed multiphysics finite element method studies to model dynamic deformations induced by laser-generated acoustic excitations. This included modal analysis, frequency domain analysis, and thermal-structural transient simulations, allowing assessment of stress and strain fields within the crystals under experimental operating conditions. The simulation results, particularly for the Acousto-Optic Modulator configuration, were used in collaboration with the MBN Research Center to conduct multiscale simulations linking FEM-derived strain profiles with molecular dynamics-based channelling and radiation emission calculations.

During the first year of the project the University of Kent, in collaboration with the MBN Research Center, conducted molecular dynamics simulations using the MBN Explorer software of Si crystals doped with Ge at levels ranging from 0 to 15% Ge at both cryogenic (10 K) and ambient (300 K) temperatures. These results show a linear dependence of lattice expansion with dopant content. The results of this work can be found in Dickers *et al.* *Eur. Phys. J. D* **78**, 77, 2024.

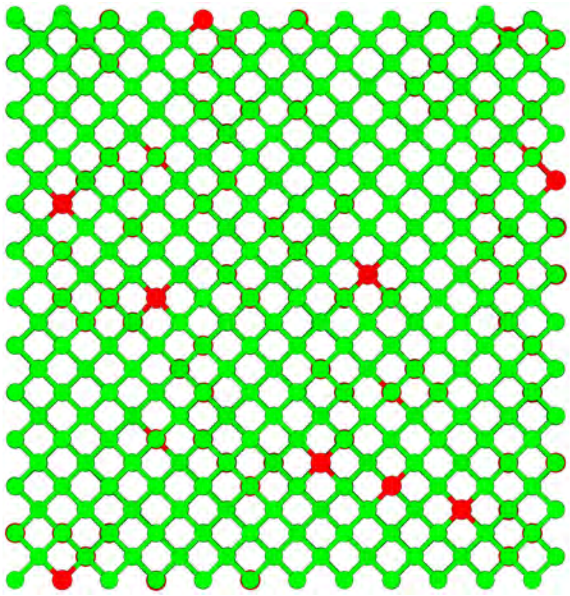

Figure 2: Illustration of a doped crystal, showing base crystal atoms (green) and dopant atoms (red).

Experimental Issues

During the first year of the project, INFN, the University of Ferrara, and the University of Padova carried out a comprehensive characterisation campaign on a range of linear, bent, and periodically bent crystals at several large-scale facilities. Measurements were conducted at the AN2000 accelerator of INFN Legnaro Laboratories and at the B16 beamline of the Diamond Light Source in the UK. This work enabled verification of crystal lattice quality and bending parameters in preparation for future experiments with sub-GeV electron and positron beams at MAMI and multi-GeV beams at CERN. It also supported the development of new Pulsed Laser Melting (PLM) techniques for germanium bending, and provided valuable data on the performance of the Diamond B16 beamline for periodically bent crystal lattice deformation characterisation.

In the first year of the project, ESRF led the initial experimental characterisation of boron-doped diamond samples intended for channelling applications. Working in collaboration with the Néel Institute in Grenoble, they produced two boron-doped diamond crystals using Microwave Plasma Chemical Vapour Deposition (MPCVD), designed with specific doping profiles to induce controlled lattice distortion along the (110) planes.

ESRF undertook X-ray characterisation of these periodically deformed crystals using high-resolution Rocking Curve Imaging (RCI) techniques. These measurements quantified the strain distributions within the crystal bulk and evaluated the uniformity of the induced deformations, providing essential structural data for subsequent modelling and simulation efforts within the project.

In the first year of the project, Uni-Mainz concentrated on experimental setup development and preliminary beamline tests for future channelling experiments. A major activity was the design and simulation of a new 500 MeV positron beamline at the Mainz Microtron (MAMI). This involved detailed studies of positron production via Bremsstrahlung in a tungsten converter, followed by energy selection, magnetic focusing, and beam transport system design to produce a low-divergence, monoenergetic positron beam suitable for CLS experiments. For more details see Backe, *et al.* *Eur. Phys. J. D*, **76**, 150, 2022.

Figure 3: *Background*: Extraction beam line of positrons at MAMI. Brown quadrupole magnets, orange dipole magnet. *Foreground*: Part of the working group.

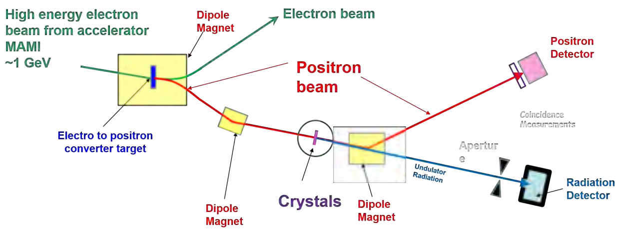

Figure 4: Illustration of the layout of the new positron beamline at MAMI.

Additionally, the University of Mainz developed and tested a calorimetric detector system using LYSO scintillators coupled with silicon photomultipliers, calibrated across a broad electron energy range at MAMI. Experimental validation confirmed positron yields and beam characteristics consistent with simulation predictions. These facilities laid the groundwork for first beam tests, demonstrating high deflection efficiency with positrons (detailed in Mazzolari, *et al.* *arXiv preprint arXiv:2404.08459*, 2024) and an initial positron channelling experiment on flat Si crystals, where beam guidance and preliminary channelling signals were successfully demonstrated in the X1 experimental hall.

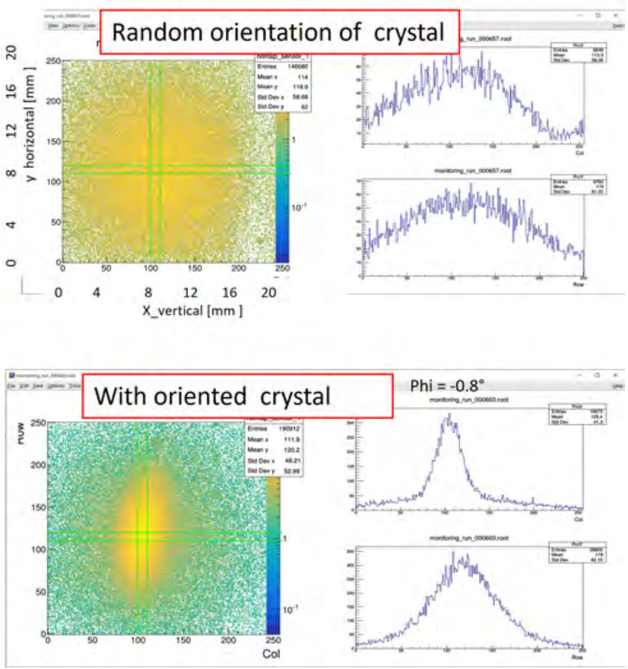

Figure 5: *Upper*: beam spot after passing a 200 µm thick, randomly orientated Si crystal. *Lower*: the same with an orientated crystal. The scattering distribution shrinks to almost the size of the original beam spot without crystal.

CLS Technology

During the first year of the project, INFN and the Univeristy of Ferrara collaborated on the development and characterisation of linear, bent, and periodically bent crystals, with a particular focus on refining surface engineering techniques for inducing lattice deformation. They prepared three linear crystals (SiC, Iridium, and Tungsten) for experimental tests at MAMI and CERN and conducted high-resolution HRXRD characterisation to verify lattice quality.

In parallel, INFN and the University of Ferrara worked with the University of Padova to improve a fabrication method for bent and periodically bent crystals based on silicon nitride deposition. This technique is particularly appealing as it allows for precise spatial control over the stress distribution imposed on the crystal, therefore allowing for fine control over the crystal bending. This involved developing a Finite Element Method (FEM) simulation model in Ansys to predict the resulting deformation profiles, and inform the fabrication of a first prototype bent crystal. The team produced such a design for a bent crystal sample, and laid the groundwork for the fabrication of periodically bent crystals using patterned silicon nitride stressor layers, setting the stage for experimental validation and further optimisation in subsequent project phases.

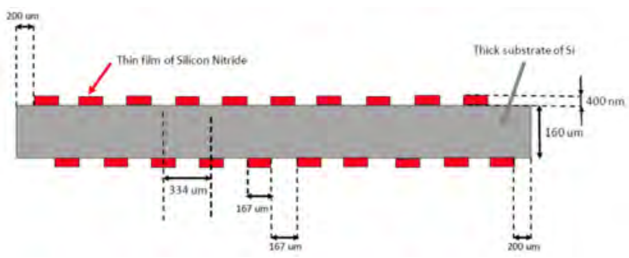

Figure 6: Scheme of the crystalline undulator manufactured using Surface Patterning by INFN and the University of Ferrara.

During the first year of the project, the University of Padova focused on the optimisation and experimental application of Pulsed Laser Melting (PLM) techniques for fabricating strained surface layers on germanium crystals, aimed at inducing controlled lattice deformation suitable for periodically bent crystal structures. Further details can be found in Carraro, *et al.* *Appl. Surf. Sci.* **509**, 145229, 2020.

Additionally, the University of Padova fabricated several $8{\times}9{\times}0.2\,\mathrm{mm}^3$ bent germanium crystals with PLM-induced stressor layers on one side, achieving a curvature radius of 15 m, verified via stylus profilometry. They performed FEM simulations to model the strain profiles and predict achievable curvature in Periodically Bent Crystals (PBCs), and began investigating patterning strategies to improve curvature uniformity and minimise higher harmonic components. These results laid the groundwork for the advanced transverse sinusoidal patterning stressor designs developed in collaboration with INFN and the University of Ferrara.

Dissemination and Outreach

In the first year of the project, dissemination and outreach activities under TECHNO-CLS were coordinated by all partners, leading to a productive start in sharing project outcomes with the broader academic and industrial communities. Across the consortium, eight peer-reviewed publications were produced, with most involving collaborative authorship between two or more project partners. A notable milestone was the preparation of a large-scale review on multiscale modelling for *Chemical Reviews*, led by the MBN Research Center and the University of Kent, which included a detailed case study on CLS technology; Solov'yov, *et al.* *Chemical Reviews* **124**, 13, 2024, which has been published during the third year of the project.

Additionally, the consortium established the official TECHNO-CLS website, managed by MBN Research Center, to serve as a central information portal for both project members and external stakeholders, and the establishment of LinkedIn[1] and Twitter (X)[2] social media pages, managed by the University of Kent, for public dissemination. The Innovation Radar identified nine innovations during this period, with at least two flagged as "business ready" and of "very high" market creation potential. Preliminary outreach to relevant companies was undertaken, with a list of 12 prospective industrial collaborators and seven CLS application partners compiled to support future engagement and commercialisation activities.

Figure 7: Participants of the TECHNO-CLS kick-off meeting on July 22-23, 2022 in Frankfurt.

[1] linkedin.com/company/techno-cls-project/
[2] twitter.com/TechnoCls

Second Year Summary June 2023 - June 2024

Theory and Modelling

In the second year of the project the MBN Research Center simulated radiation emission from 855 MeV electron and positron beams, in line with energies available at MAMI, in quasi-mosaic bent silicon crystals, predicting spectral and angular distributions of the emitted photons. The results of this study can be found in Rojas-Lorenzo, *et al.* *Nucl. Instrum. Meth. B* **556**, 2024. In addition, simulations were conducted in collaboration with both the Hellenic Mediterranean University, INFN, the University of Ferrara, and the University of Padova of positron channelling in periodically bent crystals manufactured by means of acoustic waves, surface patterning, and pulse laser melting, revealing the spectral and angular distributions of the emitted photons for various manufacturing methods.

In the second year of the project, the University of Kent extended their atomistic simulation programme to investigate structural changes and radiation emission in boron-doped diamond crystals. Using molecular dynamics simulations with MBN Explorer, the University of Kent examined how boron doping and substrate constraints influenced lattice parameters and interplanar distances in diamond, with simulations incorporating boundary conditions designed to mimic realistic epitaxial growth environments.

Additionally, the University of Kent initiated new modelling work on positron channelling in periodically bent crystals with non-harmonic bending profiles. This included mapping channelling stability under non-ideal bending conditions and highlighting limitations for crystal growth methods.

In the second year of the project, the Hellenic Mediterranean University advanced their numerical modelling of dynamically deformed crystals by carrying out thermomechanical finite element method (FEM) simulations on acoustically driven crystalline undulator prototypes. Their focus was on the Acousto-Optic Modulator-type configuration, assessing both the transient mechanical stress profiles and the thermal response in 4.3 mm-thick silicon crystals under MHz-range acoustic excitation, tailored for 20 GeV positron beams. The results confirmed that induced stresses remained within elastic limits, with peak normal stresses of 45 MPa at 350 µs and negligible thermal rise, ensuring mechanical stability of the undulator under expected operational conditions.

They also contributed to the project's multiscale modelling framework by linking FEM-derived strain fields with molecular dynamics simulations of positron beam propagation, collaborating closely with MBN Research Center to format these results for radiation emission studies. An overview of the theoretical work conducted by the Hellenic Mediterranean University in the first two years of the project can be found in Kaleris, *et al.* *Phys. Rev. Accel. Beams* **28**, 033502, 2025

In the second year of the project INFN and the University of Ferrara carried out detailed Geant4-based simulations of 530 MeV positron channelling in bent silicon crystals at the MAMI facility, reproducing experimentally observed features such as beam phase shifts and deflection efficiencies. This simulation campaign successfully validated the numerical models against experimental data and established reliable predictive tools for future positron channelling and radiation emission studies.

In the second year of the project, the University of Mainz developed and refined theoretical tools to support real-time optimisation of experimental channelling setups. They developed a custom computational code based on the continuum potential model for simulating positron trajectories and calculating radiation characteristics on-the-fly during experimental runs. The simulations take into account different assumptions about the crystal bending profile and undulator geometry, providing essential feedback for experimental alignment and parameter tuning.

Experimental Issues

In the second year of the project, the University of Mainz achieved several key experimental milestones. They completed the construction of a dedicated positron beamline at the Mainz Microtron (MAMI), which included the installation of a vacuum crystal chamber equipped with a 3-axis goniometer and an adjustable aperture system. This setup enabled precision alignment and characterisation of crystals under positron beam irradiation.

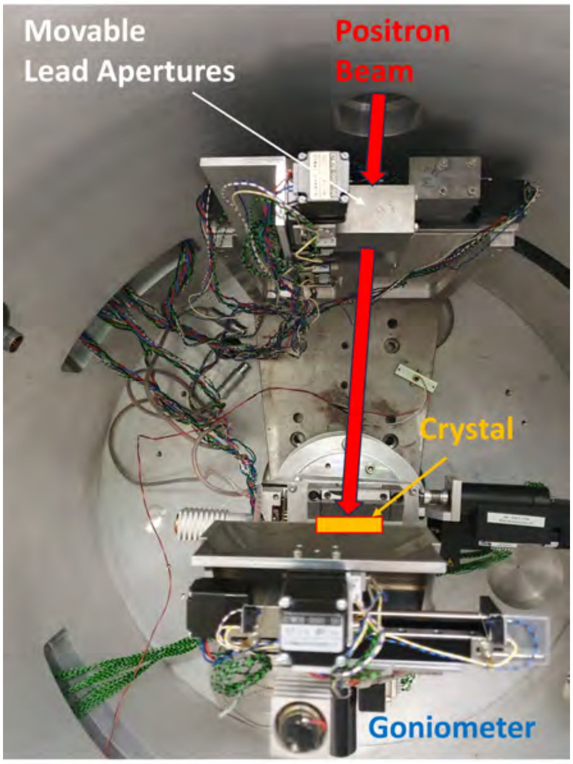

Figure 8: Vacuum chamber with goniometer and lead apertures at MAMI.

The team conducted the first channelling experiments using a 530 MeV positron beam on flat silicon crystals, successfully demonstrating clear channelling signals and achieving a channelling efficiency of approximately 60% under optimised alignment conditions. These results marked the first use of the new positron beamline for crystal channelling studies. Additionally, the University of Mainz developed a position-sensitive scintillator detector system capable of reconstructing the positron beam profile in real-time, which proved essential for optimising crystal alignment during experiments. They also advanced their work on a thermal positron source, developing a prototype magnetic transport system and electrode configuration to enable future generation and manipulation of slow positron beams at MAMI.

In the second year of the project, INFN, the University of Ferrara, and the University of Padova jointly conducted a key experimental campaign at CERN's T9 beamline in August 2023. This facility provided a tertiary electron and positron beam in the 1–10 GeV range, allowing the team to perform the first high-energy tests of radiation emission from high-Z linear crystals, specifically tungsten and iridium. The primary objectives were to characterise radiative energy loss and photon yield for multi-GeV electrons and positrons interacting with these crystals, with the data contributing both to simulation benchmarking and the planning of future tests with periodically bent structures.

Ahead of this campaign, the teams performed detailed structural characterisation of the crystal samples using laboratory X-ray diffraction and Rutherford Backscattering Spectrometry, ensuring lattice quality and defect levels met operational requirements. This groundwork enabled the successful execution of the beamline experiments, which also served as a crucial first test of beamline alignment and diagnostic systems for future CLS experiments.

In the second year of the project, ESRF continued its leadership in the structural characterisation of crystalline samples intended for CLS applications. Regular beamtime allocations at the BM05 beamline were used to perform high-resolution Rocking Curve Imaging (RCI) and X-ray diffraction measurements on boron-doped diamond crystals and other periodically deformed structures. These experiments provided precise, quantitative data on lattice strain, interplanar distance variations, and crystal rotation, enabling detailed mapping of structural quality and deformation uniformity. This information directly supported device optimisation and experimental alignment for CLS tests at MAMI and CERN.

Additionally, ESRF played a key role in characterisation campaigns conducted at the

B16 beamline at the Diamond Light Source in the UK. There, teams from INFN, the University of Ferrara, and the University of Padova performed high-precision X-ray characterisation of mechanically bent silicon crystals and newly developed periodically bent structures produced by partners using techniques like Pulsed Laser Melting. The data gathered was analysed with the assistance of INFN and verified the integrity of bending patterns, assessed dislocation densities, and confirmed the effectiveness of manufacturing techniques, providing crucial feedback for refining fabrication processes and ensuring the mechanical stability of samples in beamline conditions.

Figure 9: Examples of apparatus used for crystal characterisation. Upper: optical interferometry system. Lower: High Resolution X-Ray Diffraction system.

In the second year of the project, the Hellenic Mediterranean University developed a Mach-Zehnder optical interferometry system based on a pulsed Nd:YAG laser, enabling the precise characterisation of static and dynamic structural deformations within transparent crystalline materials. The interferometer was tested on acoustically excited Quartz crystals, successfully imaging propagating acoustic waves with undulation periods of $\sim$ 140 µm. Complementary phase imaging techniques were also implemented, and a computational model was developed to quantify acoustic pressure fluctuations inside the crystals.

In parallel, the Hellenic Mediterranean University contributed to the experimental programme by conducting a series of site visits and collaborative planning sessions at the MAMI facility in Mainz, participated in the commissioning and evaluation of the newly installed 0.5 GeV positron beamline. During this visit, they jointly designed future experimental campaigns for γ-ray generation using novel acoustically driven crystalline undulators currently in development by the Hellenic Mediterranean University.

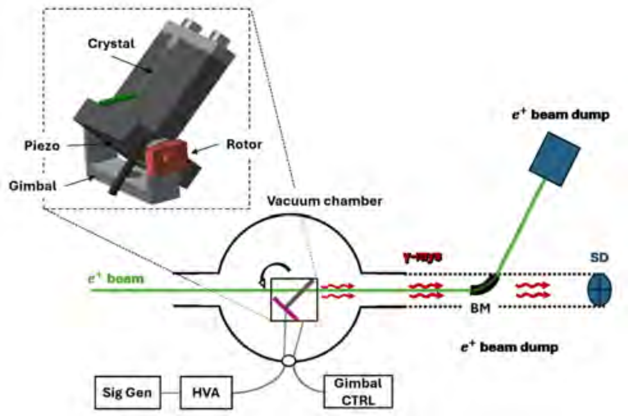

Figure 10: Schematic diagram of the experimental setup for the generation of gamma-ray radiation using an Acousto-Optic Modulator-type acoustically driven crystalline undulator.

CLS Technology

In the second year of the project, INFN and the University of Ferrara focused on further developing and refining surface patterning technologies for the fabrication of periodically bent silicon crystals. A key achievement was the fabrication of a new 4 mm long bent silicon sample using a silicon nitride stressor layer deposited on one face of the crystal to induce the desired bending. The resulting curvature was characterised using HRXRD, showing a bending of $\sim$ 60 µrad. While this sample was not suitable for CLS testing with electron or positron beams, it confirms the viability of this technique for producing bent crystals suitable for channelling applications. Futher details can be found in Malagutti *et al.* *Nucl. Instrum. Methods Phys. Res. A* **1069**, 169869, 2024.

Alongside fabrication, INFN and the University of Ferrara completed detailed finite element method (FEM) simulations to optimise the design of periodically bent crystals with a transverse sinusoidal patterning stressor pattern. This new patterning strategy was devised to minimise higher-order harmonic distortions and improve the uniformity of lattice curvature. The transverse sinusoidal patterning concept, co-developed with the University of Padova, demonstrated promising deformation profiles in simulation, and preparatory steps for photolithography mask production were completed to enable fabrication of prototype samples in the early months of the project's third year.

During the second year of the project, the University of Padova undertook an intensive research program to fabricate bent and periodically bent germanium crystals using Pulsed Laser Melting (PLM) techniques. Building on optimisation studies from the first year, this work aimed to refine the PLM process to maximise stress induced by SbGe alloy films on the Ge surface. To verify the structural integrity of the fabricated crystals, HRXRD measurements were conducted on both untreated and processed samples. These measurements quantified residual strain and dislocation densities. Additionally, the HRXRD results supplied critical input parameters for radiation emission simulations performed by other members of the research consortium, contributing to the broader goal of developing efficient crystalline undulator devices.

In parallel, Finite Element Method (FEM) simulations were performed on Ge (110) and (111) crystals processed via PLM. This modelling effort informed the practical fabrication of periodically bent crystals, where a complete process workflow was established and optimised. This included wafer thinning, lithographic patterning via direct laser writing, antimony deposition, lift-off procedures, and laser melting. The successful formation of SbGe alloy patterns and surface quality was confirmed through extensive surface analyses.

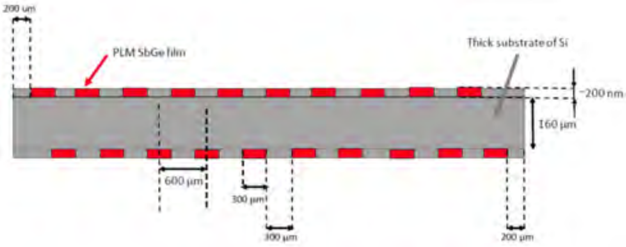

Figure 11: Scheme of the crystalline undulator manufactured using Pulsed Laser Melting by the University of Padova.

Dissemination and Outreach

In the second year of the TECHNO-CLS project, dissemination and outreach activities were significantly expanded, strengthening both the academic and industrial visibility of the consortium's work. Project partners collectively published 10 peer-reviewed articles, adding to the eight from the first year. Conference participation was also particularly active, with 27 oral and poster presentations delivered across major international conferences such as DySoN 2024 in Tbilisi and the 9th International Channelling Conference in Riccione. These presentations covered the full breadth of the project's work, from multiscale modelling and radiation simulations to experimental diagnostics and crystal fabrication techniques. Several of these contributions highlighted early results from high-energy channelling experiments and prototype crystalline undulator designs, helping to raise awareness of the TECHNO-CLS programme within both academic and applied beamline research communities.

Industrial engagement saw marked improvement in the second year. Following challenges in the first year due to external factors, the consortium hosted a dedicated TECHNO-CLS workshop in Ferrara in October 2023. This event attracted multiple industry stakeholders, including representatives from Element Six (UK), Elenos-Group (Italy), CINEL (Padova), Integra TDS (Slovakia), and experimental facilities such as STAR (Calabria), DESY (Germany), and Diamond Light Source

(UK). Discussions centred on the commercialisation prospects of crystalline undulator technologies and simulation tools, as well as potential collaborative pathways for prototype testing.

Public engagement and education initiatives were similarly expanded. TECHNO-CLS members participated in the European Researchers' Night 2023 and local Natural Sciences Festivals, promoting the project's objectives and the societal value of high-intensity, compact gamma-ray sources. To support broader visibility, the TECHNO-CLS website continued to serve as the central repository for publications, event updates, and open positions. Social media activity increased via the dedicated LinkedIn and Twitter (X) profiles, sharing conference highlights, publication announcements, and public engagement materials. The consortium also completed the integration of TECHNO-CLS into the European Commission's EIC Community and registered several project innovations for the Horizon Results Booster service, preparing for subsequent commercial exploitation initiatives as the project progresses towards prototype development.

Figure 12: Participants of the first TECHNO-CLS workshop on October 5-6, 2023 in Ferrara.