Report on the outcomes of a Short-Term Scientific Mission[1]

Action number: CA20219

Grantee name: Andrei Korol

Details of the STSM

Title: Atomistic simulations of quasi-mosaic bent crystals and their irradiation with high-energy electron beam

Start and end date: 02/10/2023 to 07/10/2023

Description of the work carried out during the STSM

During this STSM sets of data have been acquired that refer to the details on the setup of channeling experiments carried out recently at the Mainz Mikrotron (MAMI) facility (Sytov et al. *Eur. Phys. J. C* **77** (2017) 901, Bandiera et al. *ibid.* **81** (2021) 284; Mazzolari et al. *ibid.* **80** (2020) 63), to the results of measurements as well as to the details on the computational analysis of the results. In these experiments quasi-mosaic bent silicon crystals were irradiated by a collimated 855 MeV electron beam. By means of a specially designed holder the crystalline sample was bent remotely to achieve different bending curvatures and, thus, to vary efficiency of the beam steering and intensity of the radiation emitted. The following information has been collected, clarified and systematized during the STSM: (i) the parameters of the 855 electron beam used in the experiments (angular divergence and transverse beam sizes); (ii) beam-crystal alignments probed in the experiments; (iii) the measured data on the angular distribution of electrons after passing through oriented crystalline targets; (iv) spectra of the emitted radiation measured at different alignments. Apart from these, important detailed information has been obtained on geometric parameters (bending curvatures of the planar directions) of quasi-mosaic silicon and germanium crystals that were used in the aforementioned experiments as well as in those planned for the years 2023-2024. These data has appeared as the result of recent (March 2023) experiments carried out by the Ferrara team at the Diamond Light Source facility (UK) aimed at accurate characterization of the structure deformations in silicon and germanium quasi-mosaic crystals caused by external forces.

Another important outcome of the STSM concerns establishing the ranges of parameters of periodically bent (PB) crystals that will be manufactured at the Ferrara University and will be used further at in the experiments at MAMI with 600 MeV positrons (the corresponding experimental setup is currently under construction at MAMI). PB silicon crystals are produced at the Sensors and Semiconductors laboratory of the University of Ferrara by patterning the surface of a plane silicon lamina with strips in silicon nitride. Important parameters, that affect the channeling efficiency and the intensity of the radiation emitted by positrons channeled through PB crystals, are the period and amplitude of bending. Exactly these parameters have been approved so that the samples will be manufactured an used in the experiments. The corresponding numerical analysis will be carried out at

[1] This report is submitted by the grantee to the Action MC for approval and for claiming payment of the awarded grant. The Grant Awarding Coordinator coordinates the evaluation of this report on behalf of the Action MC and instructs the GH for payment of the Grant.

MBN Research center.

During the STSM, on October 5, 2023, the presentation was delivered to the group members of Prof. Guidi and Dr. Bandiera on the range of capacities and options available for multi-scale simulations performed by means of MBN Explorer and MBN Studio.

Description of the STSM main achievements and planned follow-up activities

The STSM's goal, which has been achieved, was to acquire the quantitative data and information that will allow for an independent analysis of the multiscale phenomena (multiple scattering, channeling phenomena, radiation emission) that have been investigated in recents experiments as well as that are to be investigated in the experiments planned for the years 2023 and 2024.

The follow-up analysis will be performed within the framework of the relativistic classical molecular dynamics by means of the multi-purpose computer MBN Explorer package and a supplementary special multitask software toolkit MBN Studio, which are widely exploited within the COST Action MultIChem in various research and technological areas. Accurate quantitative description of various experimental results related to the ultra-relativistic charged particles passage though bent and periodically bent crystals can be achieved provided the data on the beam parameters and crystal structure are avalable for the numerical simulations.

During the STSM it has been agreed that the results of the simulations, validated through the comparison with the experimentally measured data, will be submitted to a referred high-impact journal as a joint publication by the teams of MBN Research Center and University of Ferrara. These results will be highly relevant to the activities that are currently beeing carried out by research and technological communities towards construction of novel Crystal based Light Sources operating in the hard X- to gamma-ray ranges that can be constructed by exposing oriented crystals to beams of ultra-relativistic charged projectiles. Should such a high intensity gamma ray light source be realised then this will be important in a wide range of disciplines and have numerous potential applications.

The exploration of the aforementioned processes by means of advanced computational methods and multiscale modelling techniques directly contributes to one of the research objectives of the MultIChem COST Action and some of its tasks (e.g. WG1, T1.1), namely to development of the general multiscale methodology for modelling of the irradiation-induced processes in condensed matter systems. The knowledge obtained can be incorporated into a multiscale computational model of various condensed matter systems exposed to irradiation by high-energy electron and positron beams.