Report on the outcomes of a Virtual Mobility[1]

Action number: CA20129

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Virtual Mobility Details

Title: Atomistic Simulations of $Si_{1-x}Ge_x$ and $B_{1-x}C_x$ Crystalline Structures and their Irradiation with High-Energy Electron and Positron Beams

Start and end date: 15/09/2023 to 15/10/2023

Description of the work carried out during the VM

Description of the virtual collaboration and activities carried out during the VM, with focus on the work carried out by the grantee. Any deviations from the initial working plan shall also be described in this section.

The computational studies of crystalline structures of $Si_{1-x}Ge_x$ and $B_{1-x}C_x$ materials have been performed jointly with the group of Prof.Dr. Nigel Mason (University of Kent, Canterbury, UK). The atomistic MD simulations of the structure of $Si_{1-x}Ge_x$ and $B_{1-x}C_x$ materials have been carried out using the MBN Explorer and MBN Studio software packages [1, 2] by means of MD and the crystalline structure optimisation algorithms.

The values of the crystalline interplanar distances obtained for different concentration of the dopant atoms have been compared with the available experimental data. These results are necessary for the evaluation of the variation of dopant atoms concentration during the crystal growth process which should result in the harmonic variation of the crystalline planes in $Si_{1-x}Ge_x$ and $B_{1-x}C_x$ superlattice structures. Parameters of the manufactured superlattices will be tuned to the properties of crystalline undulators that could be realised with electron and positron beams available at the MAMI accelerator at the University of Mainz.

Simulations of high-energy electron and positron beam propagation through oriented $Si_{1-x}Ge_x$ and $B_{1-x}C_x$ superlattices have been started by means of relativistic MD. From the simulated trajectories of particles propagating through the crystalline structure an initial evaluation of the spectral and angular distribution of emitted photons has been carried out by means of the quasi-classical approach accounting for both quantum and classical effects in radiation practically within the whole range of frequencies of the emitted photons.

The obtained results are being verified against experimental measurements of various characteristics related to electron and positron beam propagation in the Si and Ge linear crystals and aforementioned

[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.

superlattices such as multiple scattering angles, dechanneling and rechanneling lengths, channeling and crystalline undulator radiation, radiation enhancement factors and others.

Such an analysis serves as an important validation of the atomistic relativistic MD and its multiscale features. It elucidates the predictive power of this simulation technique and its potential for the application in other areas of research, such as electron microscopy (where various surface structures are irradiated by beams of relativistic electrons and experience transformation in a course of such irradiation [3]), focused electron beam induced deposition (see [4] and references therein) and many more. The performed analysis is therefore providing an important example in the MultIChem Roadmap [5] aimed to be completed and published by the next annual MultiChem Annual meeting in April 2024.

[1] I.A. Solov'yov, A.V. Yakubovich, P.V. Nikolaev, I. Volkovets, A.V. Solov'yov, *J. Comput. Chem*. **33**, 2412 (2012)

[2] G.B.Sushko, I.A. Solov'yov, A.V. Solov'yov, J. Mol. Graph. Model., vol. 88, pp. 247-260 (2019)

[3] A.V. Verkhovtsev, Y. Erofeev, A.V. Solov'yov, *On the mechanisms of radiation-induced structural transformations in deposited gold clusters*, Phys. Rev. B, vol. 108, 115423 (2023)

[4] A. Prosvetov, A.V. Verkhovtsev, G. Sushko, A.V. Solov'yov, Eur. Phys. J. D, vol. 77, 15 (2023); A.V. Verkhovtsev, I.A. Solov'yov, and A.V. Solov'yov, Eur. Phys. J. D, vol. 75, 207 (2021)

[5] A.V. Solov'yov, A.V. Verkhovtsev, N Mason, I.A. Solov'yov, *et al*, *Condensed matter systems exposed to radiation: the multiscale theory, simulations and experiment*, in preparation

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

Description and assessment of whether the VM achieved its planned goals and expected outcomes, including specific contribution to Action objective and deliverables, or publications resulting from the VM. Agreed plans for future follow-up collaborations shall also be described in this section.

In this exemplar case study, it was demonstrated the feasibility of the atomistic characterisation of the above-described systems and processes therein by means of advanced computational methods and multiscale modelling techniques. This achievement 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 in this case study can be incorporated into a multiscale computational model of various condensed matter systems exposed to irradiation by high-energy electron and positron beams.

Specifically, it has been performed computational characterisation of $Si_{1-x}Ge_x$ and $B_{1-x}C_x$ materials structure (perfect and imperfect) with an atomistic level of detail; analysis of the propagation of high-energy electron and positron beams through linear Si and Ge crystals and $Si_{1-x}Ge_x$ and $B_{1-x}C_x$ crystalline superlattice structures designed for applications in CLSs; simulation of photon emission in such devices; validation of the obtained results (where possible) against experimental measurements. These results will be further validated against the results of complementary experiments to be performed at the MAMI accelerator in the University of Mainz in early 2024.

These developments are relevant to WG2 which aims to work on validation of the scientific outcomes produced by WG1 at the more complex, technology-relevant level. Specifically Task 2,4 Optimisation of computational tools for multiscale modelling for the use in technological applications related to nanofabrication and characterisation nanostructures. It will also be an example for WG3 which complements the objectives of WG1 and WG2 through inter-technology cooperation. The main goal of WG3 will be to advance the existing technological solutions through multiscale modelling.

The conducted joint research activities have strengthened the recent collaboration between the team of MBN Research Center with the Physics and Chemistry Departmental teams at the University of Kent, allowing to combine different expertise to explore the irradiation driven processes in various condensed

matter systems and the application of this knowledge in related technologies. This achievement is in line with several capacity building objectives of MultIChem, focusing on (i) Establishing a pan-European IDC community for studying collision- and irradiation-induced processes involving various molecular, biomolecular and nanoscale systems and (ii) Accumulation and systematization of the knowledge collected by different complementary communities working in the areas related to IDC.