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

Action number: CA20129

Grantee name: Leon Mishnaevsky Jr.

Details of the STSM

Title: Exploring applicability of atomistic curing models to the analysis of joining advanced composites

Start and end date: 24/09/2023 to 30/09/2023

Description of the work carried out during the STSM

The work included:

- Meeting and planning discussions with Professor Andrey Solov'yov, Dr. Andrey Korol and Dr. Verkhovtsev.
- Presentation of DTU activity in the area of computational modelling of materials science aspects of renewable energy, presentation of DTU activity in the area of bonding and curing of composites (https://youtu.be/dfJ8IWRZiMs)
- Presenting and discussing the plan of the stay. The decision was made to concentrate during this stay on application of computational mechanics methods to the deformation of materials, and linkage between deformation and wave propagation/reflection. As differed from initial planning (where direct linking between continuum and atomistic models should have been strived for), the stepwise modelling, with continuum finite element models to macroscale deformation, and analytical/atomistic model on physical effects.
- Formulations of main tasks and goals on the novel lights sources beyond free electron lasers, taking into account also particle acceleration, main goals of the study and perspectives, expected outputs,
- Installation of commercial finite element software Abaqus on the local computers, training and presentation of possibility, potential and possible application areas of finite element software to the multiphysical problems, Discussion of boundary conditions and programming possibilities for solving the Multiphysics problems,
- Development of test computational finite element models of deformation of crystals subject to light radiation, and evaluation of ray and wave propagation and reflection. Definition of loading and test boundary conditions for the crystal models and radiation interaction.
- Demonstration programming and possibilities of parameter studies.

[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.

- Planning future visit of MBN representatives to Denmark, formulation of complex multiscale finite element models, in collaboration with DTU.

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

The STSM successfully achieved its planned goals and expected outcomes. The main results of this stay include:

- With view on the COST Mission Objective “To develop specific computational workflows for multiscale modelling in nanofabrication of … composite materials”: Definition and formulation of computational finite element models of deformed crystals subject to external radiation, for the development of novel lights sources beyond free electron lasers,
- Formulation of necessary boundary conditions and loading conditions to the computational model of complex deformation of anisotropic crystals,
- linked to the COST Mission Objective: “To develop specific computational workflows for multiscale modelling…”, and “To combine and advance experimental, theoretical and computational modelling methods for studying… radiation-induced formation of nanostructures on surfaces”,
- Formulation of plans of long term future collaboration between DTU and MBN, with development of basic finite element models and more complex multiscale models, to be tested at DTU Supercomputer Cluster. Planning of the next visit of MBN colleagues to DTU, to continue the modelling and testing of anisotropic crystals. Strategy of long term collaboration between two teams, and of integration of continuum mechanical and analytical modelling of composite based light transmission, linked to the Capacity Building objective “to consolidate efforts of different research communities studying … nanofabrication methods”.

Planned follow-up activities:

- Development and validation of computational model of deforming anisotropic crystals under radiation for the optimal design of novel light sources beyond electron lasers,
- Visit to a representative of MBN to DTU and research stay at the Risø Campus, DTU Wind.
- Computational experiments at DTU and MBN; Series of complex multiscale simulations of anisotropic crystal deformation, Parameter studies.