

## Report on the outcomes of a Short-Term Scientific Mission<sup>1</sup>

Action number: CA20129

Grantee name: Elchin M. Huseynov

### **Details of the STSM**

Title: Manipulating the properties of nanocrystalline TiO<sub>2</sub> particles under the radiation

Start and end date: 11/02/2024 to 03/03/2024

### **Description of the work carried out during the STSM**

Description of the activities carried out during the STSM. Any deviations from the initial working plan shall also be described in this section.

At the present project, to investigate radiation-induced alterations of nanostructures were focused. Nanocrystalline anatase (TiO<sub>2</sub>) particles were taken as a research object. These anatase specimens were obtained in the form of nanopowder and possessed specific characteristics, including a low density 0.08 g/cm<sup>3</sup> at the nanoscale (true (bulk) density is 3.9g/cm<sup>3</sup>), extremely fine particle dimensions, each measuring less than 5 nanometers, a substantial ultra-high specific surface area (SSA) ranging from 550 to 650 m<sup>2</sup>/g, and an outstanding level of purity, with a composition purity rating of 99.9%. Powdered nanocrystalline TiO<sub>2</sub> particles were filled into high purity aluminum containers under special conditions and prepared according to the channels of the reactor. The samples used in the experiments were irradiated at full power (250kW) by a neutrons ( $5.79 \times 10^{12} \text{ n} \cdot \text{cm}^{-2} \cdot \text{s}^{-1}$ ) in channel F4 at the TRIGA Mark II light water pool type research reactor at the "Reactor Center" of the Jozef Stefan Institute in Ljubljana, Slovenia. In general, the parameters of the current neutron flux in the full power regime are regularly investigated. In total, 4 samples were divided into 4 groups and irradiated with different doses such as  $1.6 \times 10^{15} \text{ n} \cdot \text{cm}^{-2}$ ,  $8 \times 10^{15} \text{ n} \cdot \text{cm}^{-2}$ ,  $4 \times 10^{16} \text{ n} \cdot \text{cm}^{-2}$  and  $2 \times 10^{17} \text{ n} \cdot \text{cm}^{-2}$ . As a part of goals of the present STSM, radiation-induced changing of TiO<sub>2</sub> nanoparticles was investigated by ESR spectroscopy. Cooling time take few days as a result of neutron transmutation of trace elements and all ESR measurements were performed after sample activity level is suitable. The samples were filled into high-purity quartz tubes (Wilmad) with a height of 5 mm and inner diameter of 3 mm, each weighing approximately 50  $\mu\text{l}$  (1.5 mg). ESR analyzes of the samples (before and after neutron irradiation) were carried out in the BRUKER EMX II plus ESR spectrometer operated at X-band (9.85 GHz,  $\lambda \sim 3 \text{ cm}$ ). Measurements were performed at room temperature (full sweep analysis, the sweep from 500 G to 5500 G with 3300 G = 0.33 T central line).

<sup>1</sup> 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.

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

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

Present project successfully finished appropriate to research plan. All 5 working stages (WS) accomplished during experiments. Present STSM contributed to the objectives of MultiChem, as radiation-induced alterations of nanostructures. Nanocrystalline anatase ( $\text{TiO}_2$ ) particles were irradiated at the TRIGA reactor, this experiments were benefited both the MultiChem COST Action and the applicant. As an applicant aspect, he was building a new communication with reactor teams and make useful contacts with researcher in the EU. So this STEM made great collaboration for him professional aspirations. Radiation-induced morphology changes as well as impact of the paramagnetic structure and composition of metal-based NPs on their radiosensitising properties were investigated using ESR spectroscopy, which is including WG1 (T1.4). ESR spectroscopy of nanocrystalline  $\text{TiO}_2$  particles were done for 5 samples before and after neutron irradiation. Simultaneously, applicant has planned to publish article at the high profile journals appropriate to WG4 (T4.3). The nature of the new paramagnetic centers formed as a result of neutron transmutation in the anatase nanoparticles were examined by EPR spectra. As a result of neutron irradiation, the formation mechanism of  $V_{\text{Ti}}$  and  $V_{\text{O}}$  vacancies has been studied in detail. Neutron irradiations effects on the signal correspond to free electron of g factor in the EPR spectra of anatase nanoparticles were observed. An expected outcome is that, the formation of new vanadium ( $^{51}\text{V}$ ) isotopes as a result of the neutron transmutation. It is important to note that, more analytical experiments required for approving expected additional isotope. In case of formation of new  $^{51}\text{V}$  isotope and possibility control the concentration of new isotope is very important during application process. New  $^{51}\text{V}$  isotope is very useful for purposeful control of the physical properties of nanocrystalline anatase particles under neutrons. However, additional defects and other effect formation expected after neutron irradiation. In this situation more scientific experiments required for investigation neutron irradiation effects in details.