Development of A Multi-scale Material Properties and Research Data Management Workflow for Superconducting Materials

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Data management is crucial in the scope of material science digitalization and collaborative research projects. In this context, a simple modular workflow is proposed to link material properties databases with analytical and numerical modelling tools. As a first step, Python routines and Ansys Granta MI framework are used and designed to capture, curate, and manage a large amount of experimental data. Then, by means of interoperable interfaces and a simulation orchestrating platform, the data are transferred from Granta MI into a multiscale modelling workflow consisting of post-processing toolboxes and Ansys solvers to perform accurate numerical analysis. In this work, we will focus our presentation mainly on the materials data management workflow with Python routines and Ansys Granta MI. The proposed materials data management platform has been applied to study the growth and superconducting properties of bulk Sm-Ba-Cu-O superconductors fabricated in air. Various characterisation techniques have been applied, such as microstructural observation techniques including optical microscopy and scanning electron microscopy (SEM). The superconducting characterisation techniques consist of the measurement of Critical transition temperature, $\boldsymbol{T_c}$ and Critical current density, $\boldsymbol{J_c}$ by a Superconducting Quantum Interference Device (SQUID) magnetometer and trapped field scanning by a rotary Hall probe device. In addition, thermoanalytic characterisation was performed mainly by differential thermal analysis (DTA) and chemical composition analysis was achieved by a combination of energy dispersive x-ray spectrometry (EDX), X-ray powder diffraction (XRD) and electron probe micro-analysis (EPMA).

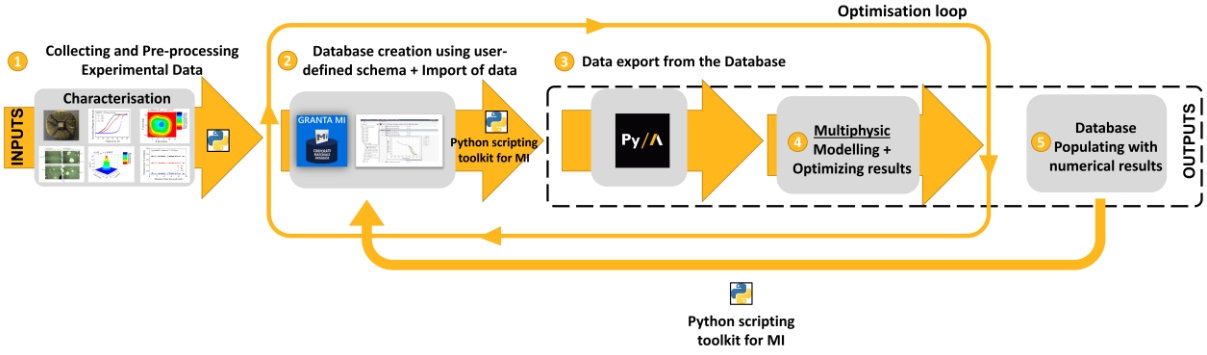

Figure 1 Illustration of the multi-scale material properties and research data management workflow