A4: Accelerated discovery of artificial minerals from machine-supported slag admixture and liquid-state processing

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Overview

Slags are byproducts of ore processing or, in a wider usage of the term, the product of smelting or melting of other raw materials, sludges and wastes. “Engineered Artificial Minerals” (EnAMs) are generated from primary slags, slag admixture and/or further additives so that critical elements can be recovered from waste (slag) streams through down-stream mechanical processing. The discovery and optimization of the formulation of EnAMs faces fundamental problems due to the complicate nature of slags. Slags are chemically complex multi-component materials outside of thermodynamic equilibrium; for this high complexity, their direct (thermodynamic or atomistic) modelling is elusive. The subproject A.4 target the problem of EnAM discovery and optimization their formulation by creating a relevant and consistent dataset and suitable descriptors, which combine physical properties and down-stream processability.

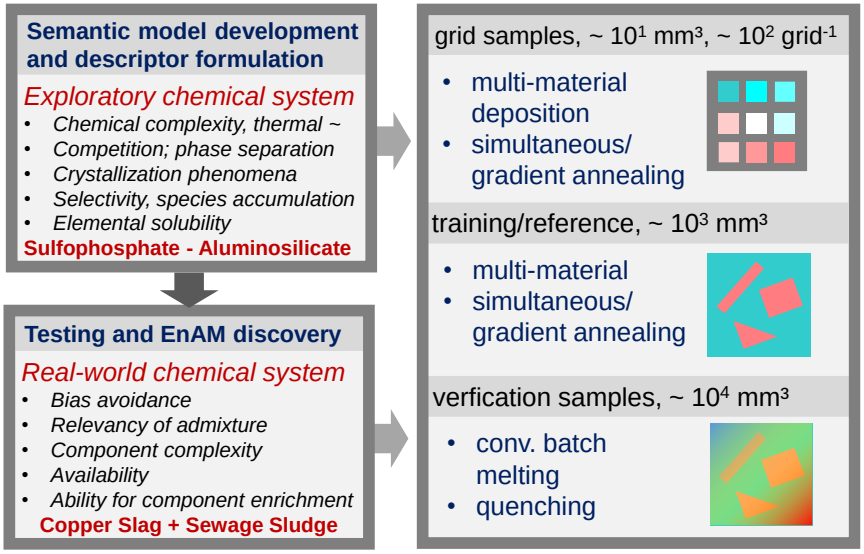

Figure 1: Schematic representation of the accelerated discovery of artificial minerals from machine-supported slag admixture and liquid-state processing.

Within this project, sample grids of up to 100 slag admixtures are produced with a broad variety of compositions, in base glass composition as well as target elements like P, Li, F and Pt-group elements, will be synthesized by high-throughput grid-printing. These sample are transferred to the liquid phase while applying spatial gradients in thermo-kinetic parameters (treatment temperature, timescales and cooling rates) in order to probe EnAMs with variable microstructure (induced by variations in the solidification and crystallization process). By following applied analysis techniques, the materials will be characterized regarding chemical, structural und mechanical properties, especially regarding the distribution of target elements on the (intentionally) formed phases and their down-stream processability. The holistic descriptors are conceived from this physical data The EnAM discovery ability of the dataset and descriptors are verified by the real world chemical system of copper slag and sewage sludge.