Closing the Microstructure-Quantification Loop with SMART (Spatial Mapping And Robust Thermomagnetics)

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Correlating local microstructure with macroscopic functional properties remains a bottleneck in materials design [1]. Fully automated segmentation of SEM and EDS data suffers from stereological bias: interaction volumes overlap at phase boundaries, illumination varies across the field of view, and chemically distinct magnetic phases can show nearly indistinguishable Z-contrast. In Sm–Fe–V the 1:12, 3:29 and 2:17 phases differ by only ~1–2 at.% Sm, too narrow to resolve by contrast alone.

We present SMART, an open-source, human-in-the-loop framework that closes this loop (Figure 1). A Random Forest [2] classifier trained on sparse annotations over a texture-based feature stack stays robust to illumination gradients and polishing artifacts, and redeploys across image series. Phase identities follow from stoichiometric rules held in external JSON files rather than source code, and area-weighted per-phase compositions reconstruct the bulk. An independent module extracts Curie temperatures from $M(T)$ curves by automated dual-tangent intersection, an objective physical anchor for magnetic phase assignment, while an Isolation-Forest [3] anomaly map flags unclassified regions, so a phase seen magnetically but missed spatially can be located and annotated. The modules are decoupled: each runs standalone, and together they merge into one correlative database linking phase fractions, chemistry and magnetic transitions.

Across 24 Sm–Fe–V ingots and 80 micrographs, reconstructed and measured bulk compositions fall on parity, as do segmented and Rietveld phase fractions. Where they diverge the cause is preparation: ductile FeV resists grinding and is retained in the sieve, so XRD underestimates it. Working on polished cross-sections, SMART avoids this bias, resolves trace and non-crystalline phases invisible to bulk scattering, and unlike Otsu or K-means does not read illumination gradients as phases. The loop also drives discovery: thermomagnetic detection of a phase absent from an initial segmentation guides annotation of the regions the anomaly map flags, after which residual risk collapses to the phase boundaries alone. Needing no annotated training corpus and shipped as a zero-code executable, SMART is openly available at https://github.com/aarondexz/SMART.

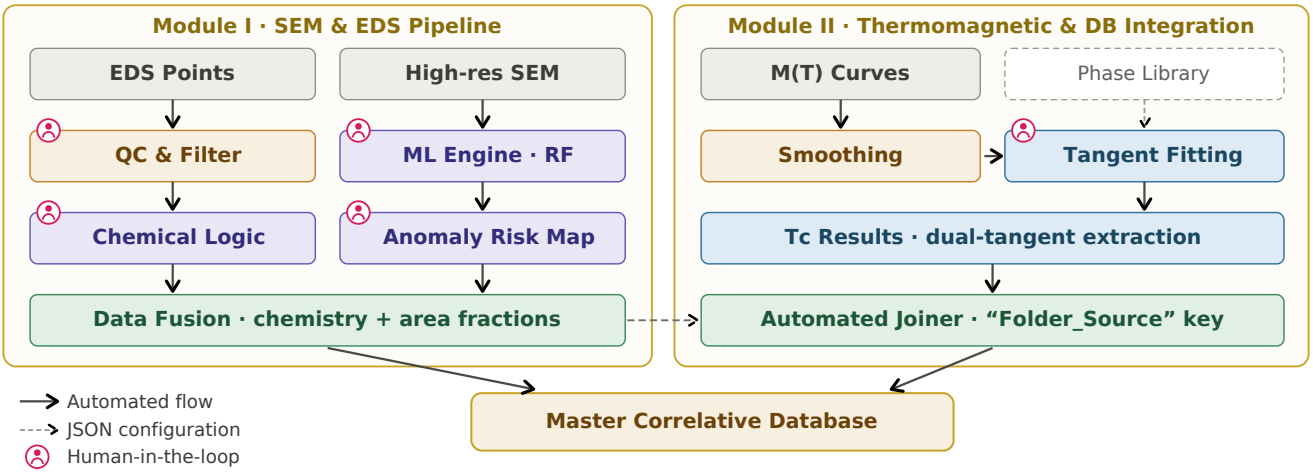

Figure 1: The SMART correlative workflow. Module I segments SEM–EDS data with a Random Forest, assigns phases from JSON stoichiometric rules and flags unclassified regions with an Isolation-Forest anomaly map; Module II extracts Curie temperatures from $M(T)$ curves by dual-tangent fitting. Badges mark the points of human-in-the-loop intervention. The modules run independently or join into one correlative database.

References

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