PHASES Agent: an AI agent for physics-based digital metallurgy

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Predictive metallurgy is often promised and rarely delivered. Most tools stop at a property lookup or a single calibrated model, and the few that reach further tend to stay inside a specialist's script. Phases (https://phases.aerobase.se), built by Aerobase Innovations AB, works differently. It is an AI agent that runs physics-based phase-transformation models from a plain-language request and returns a finished simulation with plots, and it already drives a validated automotive process chain from hot forming through welding to crash. This abstract describes the platform and the physics behind it, then shows the result that makes the case: a single composition-dependent model, applied across a full press-hardening chain, predicts how the chemistry of recycled steel changes crash performance.

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Inside PHASES

The platform brings together three capabilities that typically reside in separate systems. The first is a digitized materials database: CCT, TTT, and TTP diagrams covering the most common steels and non-ferrous alloys, along with hundreds of flow-stress data sets that contain thousands of curves across various alloy families. An OCR pipeline reads legacy diagrams and extracts critical temperatures (Ac1, Ac3, Ms, Bs), cooling curves, corresponding hardness values, and phase boundaries from scanned images, converting decades of published metallurgy into data that an engineer can filter by alloy composition.

The second is PHASES, the composition-dependent phase model at the platform's core. It couples Koistinen–Marburger [3] martensite kinetics with diffusional transformation models [4] that depend on grain size, chemistry, and deformation history, and it predicts local phase fractions and the resulting mechanical properties as composition changes. Because the critical temperatures (ex A_{e1}, $A_{e3,}$ B_s, M_s), activation energy, initial yield stress, and failure strain are expressed as functions of chemistry, a single model can predict the phase kinetics during heating and cooling rather than being refitted at each temperature cycle. The same model also adapts to changing alloy chemistry rather than a fixed grade, and the aim is to extend it into a unified description of phase transformation that spans both steels and non-ferrous alloys — the database already covers both.

The third is the agent. An engineer asks for a CCT diagram, a spot-weld nugget, or a heat-treatment response in ordinary language; the agent selects the model, runs it, stores the results, and returns the plots. None of the underlying solver setup needs to be done by hand.

Validation in the CiSMA project

Whether a tool is valid depends on its performance on an actual part. In the EU Horizon Europe project CiSMA, PHASES was tested on a full press-hardening process in LS-DYNA: hot stamping of a 22MnB5 hat profile with tailored soft zones, resistance spot welding to a DP780 cover plate, and axial crushing of the assembled parts. One composition-dependent model monitored microstructure and properties from forming through re-austenitization, tempering in the weld heat-affected zone, and into crash analysis. Testing various compositions with realistic electric-arc-furnace scrap fractions revealed how residual elements — Mn, Si, Cr, Cu, and Sn — influence phase fractions after stamping, affect nugget growth during welding, and cause variations in force–displacement responses during crushing. This provides a direct way to evaluate circularity: ensuring that higher-scrap grades still meet crash performance targets before casting a heat.

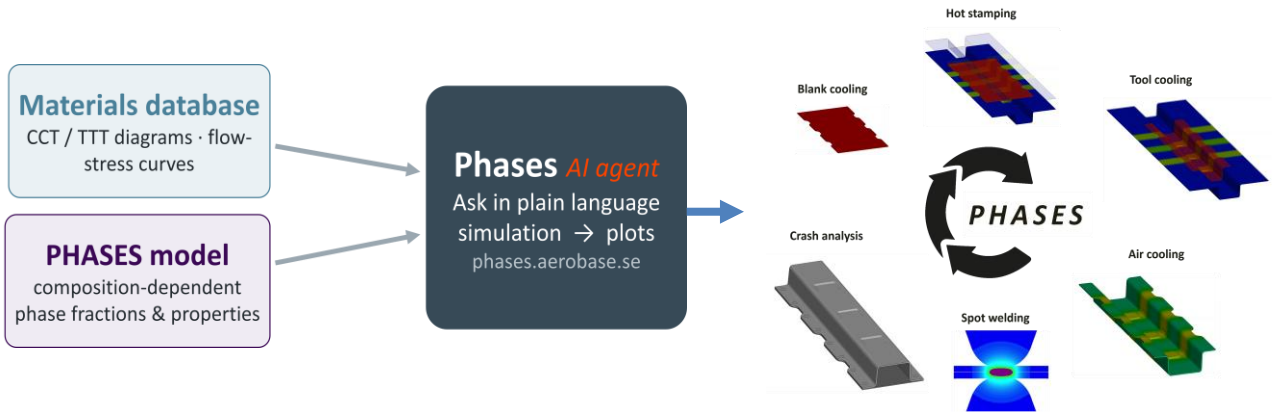

Figure 1: PHASES — a digitized materials database and the physics-based PHASES model, reached through an AI agent and applied across the validated CiSMA forming–welding–crash chain.

Where this sits, and what we will show

Most current AI-for-steel efforts focus on the front end of the materials lifecycle: data-driven models that accelerate alloy discovery and propose the next composition to test. PHASES works at the other end. It predicts how a given steel behaves in a general thermal cycle, keeping the physics in view so that answers trace back to transformation kinetics. An engineer reaches it through a conversation and gets a concrete result by running an online simulation of a given thermal cycle, spot-welding, or heat-treatment case, or by exporting a material card to a commercial or open-source FE program.

At ESTEP 2026, we will run the PHASES agent live: querying the diagram database, generating CCT/TTT and spot-weld predictions from composition, and stepping through the CiSMA crash results for several scrap-driven compositions. The contribution falls within predictive modelling and digital metallurgy, integrating physics-based and AI-based microstructure–property modelling with process–property–performance integration in a tool that already runs.

References

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