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Review paper

INTEGRATED COMPUTATIONAL MATERIAL ENGINEERING PRACTICE PATHS BY CHANGSHA RUIRUI TECHNOLOGY: FROM CALPHAD TO PHASE FIELD AND CRYSTAL PLASTIC FINITE ELEMENT

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Abstract

This work presents a digital workflow and a suite of integrated software tools developed by Changsha Ruirui Technology Co., Ltd. for the design of metallic materials within the Integrated Computational Materials Engineering (ICME) framework. The platform seamlessly connects CALPHAD-based thermodynamic and thermophysical property calculations with phase-field microstructure simulations and crystal plasticity finite element analysis. Key in-house developed software—including ICALPHAD, CALTPP, MID-MESO, PRECALC, and CPCP—are introduced, emphasizing their interoperability and data transfer capabilities. The application of this integrated approach to an Al-Mg-Si alloy successfully predicted mechanical properties by accounting for critical microstructural features such as precipitates, texture, and grain size, demonstrating its significant potential for accelerating the development of advanced structural materials.

***Keywords**: ICME; multiscale modeling; software integration; microstructure; mechanical properties*

1. INTRODUCTION

Integrated Computational Materials Engineering (ICME) has emerged as a transformative paradigm in materials science, aiming to unify material design, manufacturing, and performance prediction through integrated multiscale modeling and simulation [1]. A cornerstone of ICME is establishing the "process-structure-property-performance" linkage. However, a significant challenge lies in effectively integrating disparate computational tools across various scales to ensure robust data transfer and theoretical consistency.

To address this challenge, a digital workflow was developed based on the "microstructure-performance correlation". It starts from scientific databases and integrates phase diagram thermodynamic calculation, thermophysical property calculation, phase field simulation, and crystal plasticity finite element calculation in sequence. For each computational stage, dedicated software tools were designed and developed. These developments focused not only on solving specific computational problems but also on ensuring theoretical connections and seamless data transfer between them, aiming to create a universal intelligent design platform for metallic structural materials, as depicted in Figure 1.

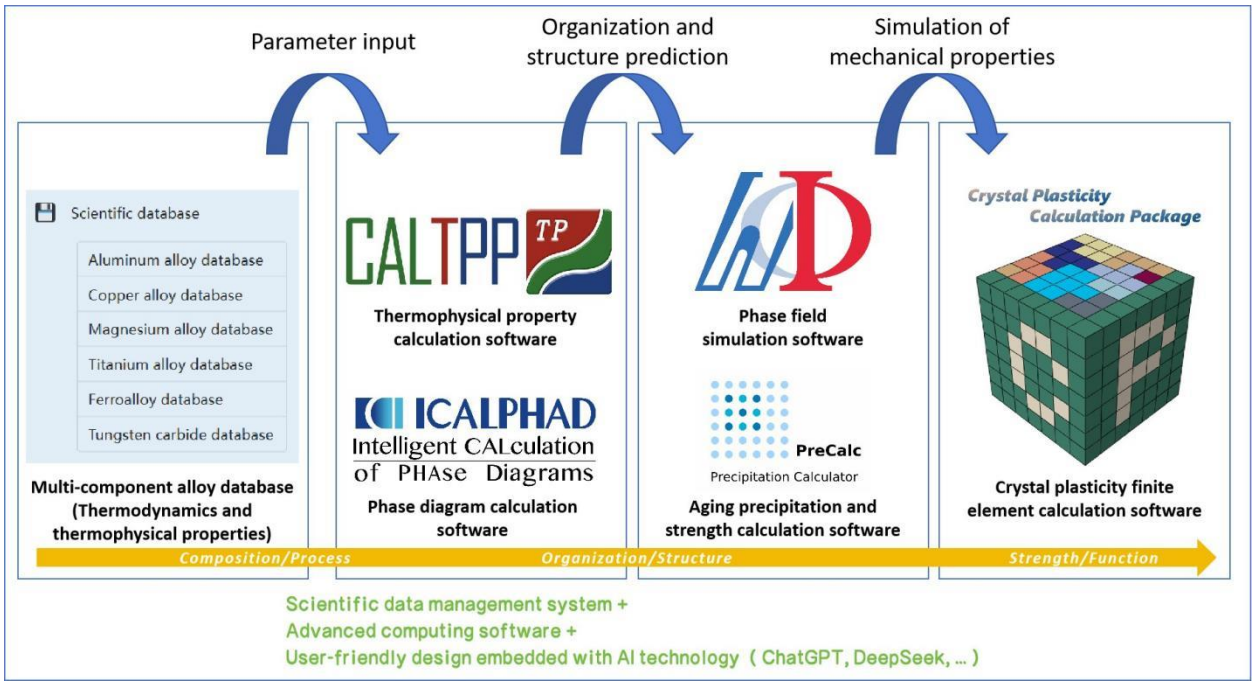

Figure. 1 ICME flowchart based on database and software

2. METHOD

The digital workflow consists of several sequentially linked computational modules, each implemented through dedicated software tools. The software in the Fig. 1 is briefly introduced as follows:

ICALPHAD (Intelligent CALculation of PHAse Diagrams) [2]:

A software tool based on the CALPHAD method for calculating phase diagrams and optimizing thermodynamic parameters of materials systems. It is used for predicting material properties and phase behavior in materials science and engineering. For more information, https://doi.org/10.1016/j.calphad.2025.102810.

CALTPP (CALculation of ThermoPhysical Properties) [3]:

Provide various thermophysical properties such as diffusion coefficient, interfacial energy, thermal conductivity, viscosity. For more information, https://doi.org/10.1016/j.jmst.2019.12.005.

MID-MESO (Microstructure Intelligent Design MESOscale) [4]:

An open-source phase-field solver package for simulating multiphase transformation and mechanical analysis of polycrystalline nanoparticles. For more information, https://github.com/Microstructure-Intelligent-Design.

PRECALC (PREcipitation CALCulator) [5]:

A computational software for age-hardening materials, integrating functions such as age precipitation and macroscopic strength and electrical conductivity prediction. For more information, https://doi.org/10.1016/j.jmrt.2024.05.145.

CPCP (Crystal Plasticity Calculation Package) [6]:

A research/teaching toolkit based on the crystal plastic finite element method. At present, it has successfully carried out calculation simulation on aluminum alloy, high-strength steel, cemented carbide, coating materials and so on. For more information, https://www.ams.org.cn/CN/10.11900/0412.1961.2024.00083.

3. RESULTS AND DISCUSSION

This series of software components involved in the workflow encompasses the transmission and circulation of various material information.

Starting from the database, phase diagram information and thermophysical data of alloy materials at specified compositions and temperatures are obtained through ICALPHAD and CALTPP software, which supports the subsequent phase field simulation (MID-MESO) and precipitation prediction (PRECALC).

After obtaining the exact state of the structure and microstructure, the mechanical property prediction under specified loads is conducted through crystal plasticity finite element software. Figure 2 shows the corresponding computational steps behind the combination of these software.

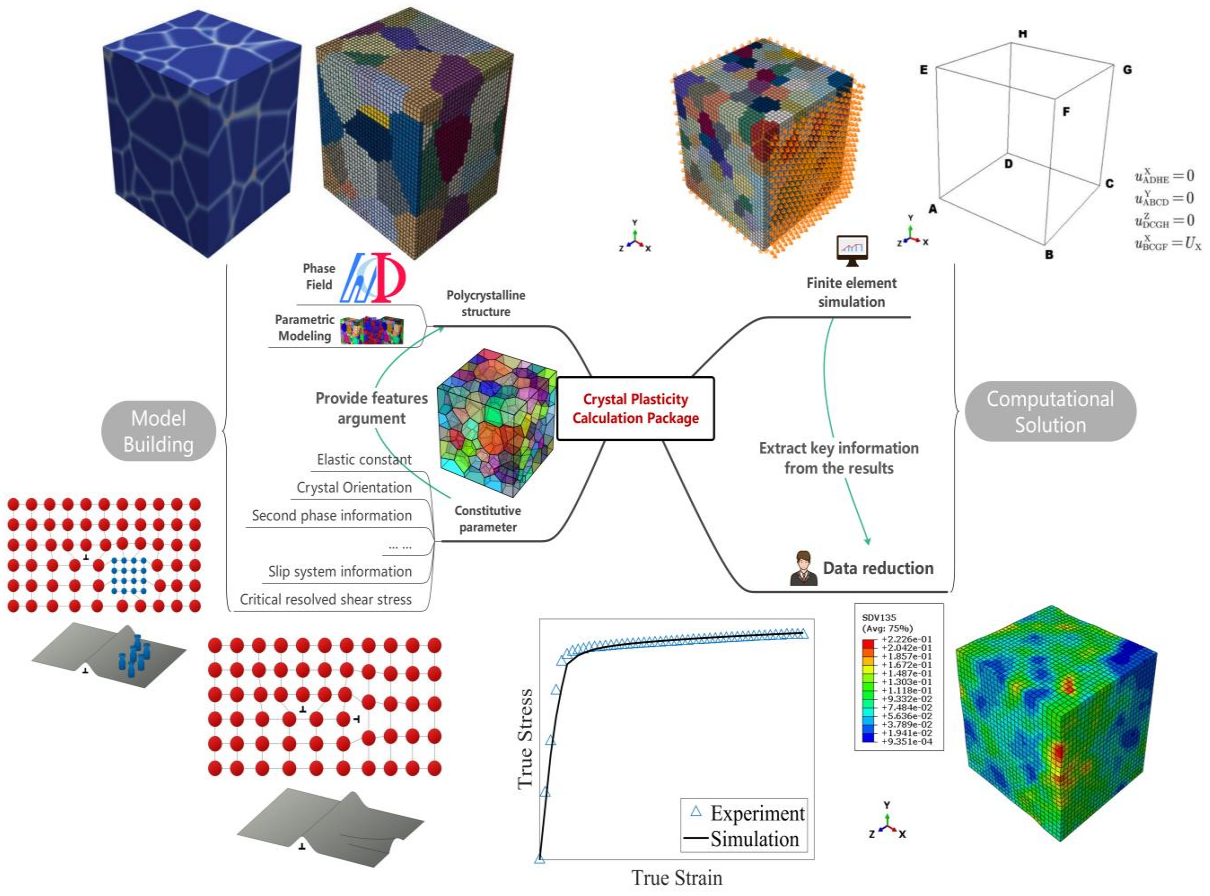

Figure. 2 Flowchart of crystal plasticity finite element calculation

Figure 3 demonstrates the application of this work in Al-Mg-Si alloys [6], where the strength and toughness are closely related to the precipitates.

Moreover, factors such as texture, grain size, and the content of solid solution phase also play significant roles in the mechanical properties of the material, which highlights the advantage of integrated computing in considering multiple microstructural features.

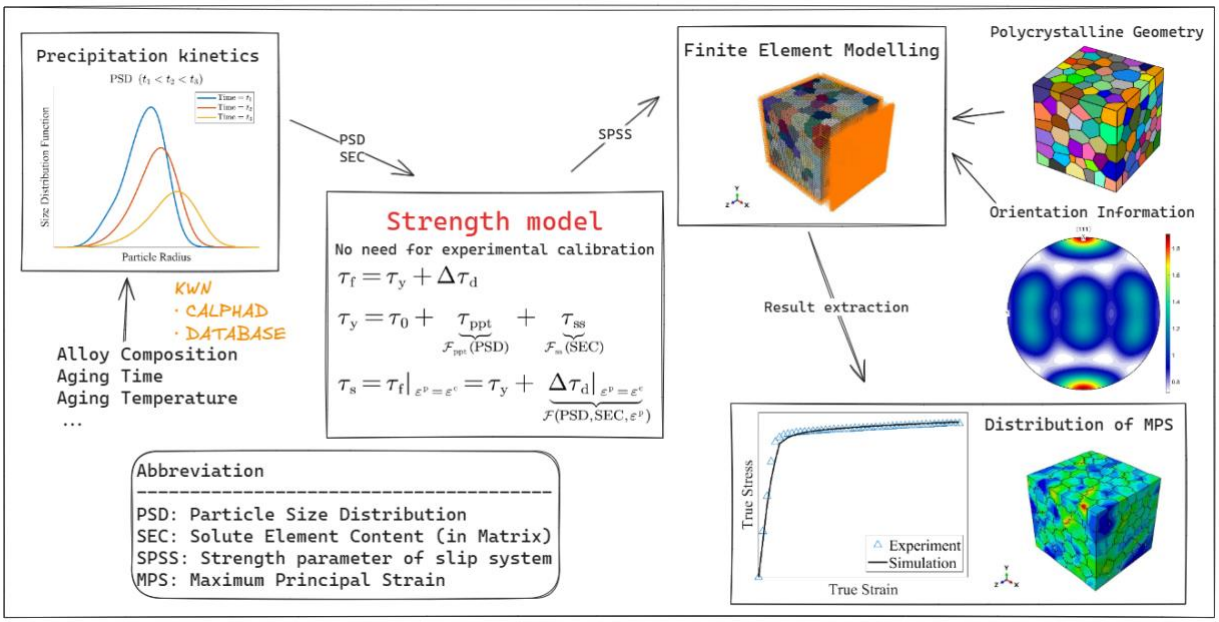

Figure. 3 Integrated calculation of aging precipitation, strengthening and crystal plasticity finite element simulation of Al-Mg-Si alloy

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