CALPHAD-Supported Materials Design: Case Studies and Challenges

Jiayi Yan
Department of Materials Science and Engineering, KTH Royal Institute of Technology,
Brinellvägen 23, 10044 Stockholm, Sweden

Abstract

CALPHAD toolsets and databases represent Materials Genome with arguably the highest degree of sophistication and readiness for computational materials design. Born to describe equilibrium phase relations, CALPHAD has been extended to cover non-equilibrium phases and physical properties. Ab initio calculations are also embraced by CALPHAD with necessary scrutiny. The success of materials design relies on the maturity of CALPHAD, and reversely the design practice brings challenges to CALPHAD. This is elaborated using the case studies that the presenter has been involved in at Northwestern and KTH, including design of transformation-toughened Ti alloy and medium-Mn steel. Challenges to CALPHAD related to these projects include metastable/unstable phase stabilities, short-range order, α” martensite and ω’ phase in Ti alloys, and carbon-defect interactions in ferrous martensite.