THERMODYNAMIC AND KINETIC MODELING TOOLS AND THEIR APPLICATION TO THE LIFECYCLE OF STEELS

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Abstract

Computational thermodynamics, such as the CALPHAD (CALculation of PHAse Diagrams) method, has evolved over the past four decades to become a powerful, flexible tool for the study of a variety of scientific and technological areas of industrial importance. For example, it was rather early on successfully applied in alloy development for steels, and has since then continuously developed towards use in more and more applications within the lifecycle of steels. Computational kinetics software tools, such as DICTRA which simulates diffusion controlled reactions based on numerical solution of the multi-component diffusion equations, and TC-PRISMA which treats concurrent nucleation, growth/dissolution and coarsening using Langer-Schwartz theory and the Kampmann-Wagner numerical approach, are today also successfully applied within several areas of the lifecycle of steels.

This presentation aims to describe some recent advances in the application of computational thermodynamics and kinetics to complex situations within the lifecycle of steels, ranging from alloy design to scrap re-cycling. For example, applications in the R&D stage can be found in pre-screening potential candidate compositions to guide experiments more efficiently, and in optimizing the operational conditions, etc. Applications can also be found in predicting phase formation and determining the sensitivity of a particular property for quality control; simulating the nucleation and growth of precipitates during heat treatment; predicting liquidus temperature from mixing scrap metal of different compositions and predicting reactions during combustion of waste for the application of waste and re-cycling. In the present work, selective application examples in casting, forging/rolling, heat treatment, joining/welding, corrosion and failure analysis will be demonstrated.

Keywords: Computational thermodynamics, kinetics, steels

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