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INVITED LECTURE

COMPUTATIONAL DESIGN OF ENGINEERING MATERIALS: CASE STUDIES FOR A CEMENTED CARBIDE AND A HEAT RESISTANT ALLOY

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Abstract

A brief overview of state-of-the-art in the field of computational design of materials is given. It comprises multi-scale computational methods such as CALPHAD, atomistic simulations, phase-field and cellular automaton, and crystal plasticity finite element analysis. In the second part of this presentation, case studies for design of a gradient cemented carbide [1] and a heat resistant high-strength Al alloy [2] are presented. They are considered from the point of view of a step-by-step application of the basic methods. It is suggested that disseminating [2] this approach among professionals and students will enhance accelerated design of materials and their processing.