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METHODS
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Preface

The wide use of alloys, particularly bronze, iron and steel, has characterized the advancement of human civilization. By combining a metal with other chemical elements to form an alloy, the resultant material may achieve properties that are superior to those of the individual constituents. Consequently, alloying provides a flexible way to find or create new materials with better performances, like specific strength/stiffness, hardness, fracture toughness, fatigue life, wear resistance, as well as thermal, electrical, or magnetic characteristics. Nowadays, alloys form a large family of metallic materials that play a significant role in advanced technologies, such as building, transportation, aerospace, microelectronics, energy harvesting/storage, precision instruments and machinery.

Traditionally, experimentation was the main approach to studying the properties of alloys and developing new ones. With the rapid growth of computational capability, research and development on advanced alloys increasingly relies more on computational methods, significantly saving both time and costs. Computations can reproduce, at least to some extent, the material's physical process and its microstructures during fabrication and manufacturing, thus providing tremendous support for the design and optimization of advanced alloys and related structures.

A variety of computational methods meet the demands for numerical representation of the material behaviour at different scales, such as first principle calculation, molecular dynamics, cellular automaton, phase field modelling, micromechanical modelling, and finite element method. The latest developments in the computational research on advanced alloys urged the editor to invite recognized authors in this field to submit papers to this special issue of the "Computer Methods in Materials Science" journal.

The finite element (FE) method is currently the dominant method for numerical analysis of the macroscopic physical behaviour of solid materials and structures. It is established on a continuum base, and the material behaviour is described by a constitutive model, whose accuracy is significantly affected by the yield model. Wang et al. conducted uniaxial and biaxial tensile tests to obtain the yield loci of an ultra-thin austenite stainless steel. The Yld2000 yield model was calibrated using the yield loci under different equivalent plastic strains to optimize the prediction accuracy for the springback and thickness distribution.

Jiang and Xiao dealt with the constitutive modelling of superelastic NiTi shape memory alloys and its implementation in FE software, based on which the localized deformation, fracture and thermomechanical coupling can be numerically reproduced and analyzed. Innovatively, parametric studies were performed to unveil the effects of grain size, transformation hardening modulus and yield stress on the physical properties of the material.

Micromechanical models rely on micromechanics to obtain an expression for the interaction energy within the material. Xiao et al. proposed a temperature-dependent micromechanical model of a superelastic NiTi shape memory alloy by considering 24 transformation systems and the associated cycling-induced degradation of superelasticity. The scale transition was accomplished numerically by FE techniques to account for the complex interaction between neighbouring grains. The mechanical responses under cyclic tension and bending were predicted and discussed.

In summary, the collected papers clearly show the capabilities and contributions of computational methods to the research of advanced alloys, and readers have an excellent opportunity to take a look at what is happening on the frontier of the numerical modelling of materials.

Yao Xiao
Guest editor