Preface

This special edition is dedicated to advances in computational materials science and modelling approaches that underpin the understanding and prediction of mechanical properties, behaviour and microstructure of modern materials. The investigations span micro- and macro scales, integrating continuum mechanics, statistical modelling, and microstructure-based theories with crystallographic texture, dislocation mechanics, and recrystallisation phenomena. Established and emerging models—such as the Mori–Tanaka scheme, Kocks–Mecking framework, Smith–Zener drag mechanism, CALPHAD-based modelling, phase-field methods, and diffusion theories—are applied to complex materials including aluminium and vanadium alloys, hexagonal titanium, aluminium matrix composites, bulk metallic glasses, and additively manufactured metals.

The edition further highlights first-principles computations, molecular dynamics simulations, finite difference and finite element analyses for evaluating phase stability, segregation energy, residual stresses, and grain size distribution. Processing routes such as copper mold casting and spark plasma sintering are examined alongside microstructure evolution, phase coarsening, and additive manufacturing. In addition, data-driven approaches, including machine learning and materials informatics, are presented as powerful tools for accelerating materials design and microstructure modelling.

This edition offers a comprehensive and forward-looking perspective on theory-driven and computationally assisted materials engineering, providing valuable insights for many specialists in materials science.