Special Issue

Molecular Dynamics Study of Metal Alloys

Message from the Guest Editors

The optimization of metal alloy compositions is a practical route to achieve the target strength and stiffness of materials for engineering applications. Molecular dynamics (MD) simulations with an appropriate choice of interatomic potential can provide unprecedented details of the behavior of materials, elucidate the dynamics of defects, and fracture mechanisms. The recent advances in the development of interatomic potentials and high-performance computing facilities enabled *in silico* discovery of new alloy compositions with extraordinary mechanical properties and unraveling the structure-property relationships to guide their experimental synthesis. In particular, the design of the emerging class of materials such as shape memory alloys (SMA) and high-entropy alloys (HEA) can heavily benefit from the *a priori* prediction of the strength and related properties from the MD simulations. The Special Issue is focused on "Molecular Dynamics Study of Metal Alloys", with the aim to collect original research articles and scientific reviews highlighting cutting-edge and innovative scientific advancements and future directions in this field.

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About the Journal

Message from the Editor-in-Chief

Metallic materials play a vital role in the economic life of modern societies; contributions are sought on fresh developments that enhance our understanding of the fundamental aspects related to the relationships between processing, properties and microstructure – disciplines in the metallurgical field ranging from processing, mechanical behavior, phase transitions and microstructural evolution, nanostructures, as well as unique metallic properties – inspire general and scholarly interest among the scientific community.

Editor-in-Chief

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