DATA-DRIVEN AND COMPUTATIONAL MATERIALS DESIGN

Chemistry and Physics of Interfaces

Understanding the chemistry and physics of interfaces is central to controlling and predicting materials behavior. While the broad importance of interfaces to materials science has long been appreciated, ongoing developments in materials modeling coupled with advances in micro- and nanoscale characterization methods, continue to yield new discoveries and insights into the elementary mechanisms by which interfaces evolve and mediate materials properties. As we learn more about interfaces, it is becoming increasingly clear that the behavior of interfaces cannot be understood solely in terms of their isolated ground-state behavior. Instead, we must also consider a diversity of stable and metastable interfacial states, the barriers between them, and their interactions with other point, line, and chemical defects.

This symposium aims to bring together experimentalists and materials theorists researching the fundamental science of interfaces in materials. The symposium will consider several different classes of interfaces, including grain boundaries, crystalline interphase boundaries, surfaces, and boundaries between crystalline and amorphous phases (including solid/liquid interfaces).

Topical areas of interest include but are not limited to:

• Mechanisms underpinning interfacial motion including grain evolution and phase transformations.
• Compositional effects, including effects on interfacial chemistry, effects on mechanisms and kinetics of phase separation, effects of alloying on interface energy, effects of strain on interfacial diffusion processes.
• Approaches to engineering and tailoring interfacial properties, linking fundamentals of interfacial structure, processing, and behavior at various length scales (e.g., tailoring dopant segregation, electronic/magnetic modulation, orientation/texture engineering).
• Response of interfaces to strain, including interactions with point defects and line defects such as dislocations, disconnections, and boundary junctions.
• Mechanisms of interfacial response and stability in extreme environments (including irradiation exposure, temperature extremes, corrosive conditions, and effects of pressure and stress in microstructure and properties).
• Advanced data science methods, particularly where the methods elucidate new foundational insight from large interfacial experimental or modeling data sets.

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