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Editorial: Modeling of structural and chemical disorders: From metallic glasses to high entropy alloys

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Editorial on the Research Topic
Modeling of Structural and Chemical Disorders: From Metallic Glasses to High Entropy Alloys

Complex materials such as metallic glasses (MGs) and high-entropy alloys (HEAs) have received considerable attention over the past few decades (Ma and Wu., 2019; Qiao et al., 2019), because: 1) their inherently disordered local structures and chemistries provide a rich variety of environments as the ideal playgrounds and testbeds to examine the most fundamental questions in materials science, namely the structure-property relationship; and, 2) the metastability nature has endowed them with great potentials for properties control and subsequently numerous engineering applications.

While tremendous progresses have been made in the field, formidable challenges still exist that have hindered a predictive and fundamental knowledge on the mechanical and physical behaviors in MGs and HEAs. In particular, the challenges mainly come from two aspects: First, effective and robust structure-property relations are very difficult to be built in these materials with strong structural and chemical disorders; Second, as non-equilibrium systems, MGs' and HEAs' structures and properties are dynamically evolving, subjected to the processing histories and operational conditions. In recent years new concepts and algorithms—including short/medium range orders, i.e., SROs/MROs (Ding et al., 2018; Xing et al., 2022), energy landscape quantifications (Fan et al., 2014b; Cao et al., 2019; Liu and Fan., 2021), structural heterogeneities (Fan et al., 2014a; Ding et al., 2014), atomic-level stresses fluctuations (Iwashita et al., 2013), *etc*—have been proposed and shown promising progresses. Within such a context, we present a salient Research Topic of research papers in this Research Topic, which shows some novel and important results in the field.

Shen et al. employed different processing protocols in molecular dynamics simulations to produce two different packing structures, namely a homogeneous liquid-like L-phase glass by rapidly quenching a high-temperature equilibrated liquid, and a sub-T_m annealing treated heterogeneous solid-like G-phase glass with short-range crystal-like order embedded in a liquid-like matrix. It is found that, even under the same global composition, the plasticity in G-phase glass mainly consists of mechanical-induced regional melting of icosahedral-featured space within narrow shear band, while the deformation in L-phase glass is more diffuse.

Shiihara et al. employed first principles method to probe the origin of atomic-level stresses in FCC and BCC HEAs. Within the random solid solution states, a strong correlation is observed between the experimentally estimated yield stress and the atomic-level pressure dispersion. It has been further demonstrated that, the atomic-level pressures in FCC HEAs originate from charge transfers, while in BCC HEAs the atomic volume differences play a decisive role. These findings thus provide important atomistic insights into harnessing the strengthen of complex alloys consisting of multiple principal elements.

Gu et al.; Shen et al. combined both experimental measurements and computational modelling to probe the role of nanoscale structural heterogeneity in the dynamic mechanical performance (e.g., strain rate sensitivity, SRS) in MGs. They established a mechanism map of deformation to explain the SRS and deformation patterns with the consideration of various processing histories and testing conditions. The obtained insights from this study may pave the way to design the nanostructured MGs for desired dynamic applications.

Yang et al. reported a novel physics-informed structural parameter, which is reflected by the ergodic, and atomic packing diversity that an atom fluctuates for sufficiently long time. Such Shannon-information-entropy-inspired parameter does not only enable the accurate prediction to elementary structural excitations' activation barriers, but also establishes a correlation with MGs' boson peaks. They concluded those findings shed light on advancing the robust and accurate atomic-level structure–property relationship in amorphous materials.

The contribution of Wang et al. focused on doping oxygen into a ferromagnetic Co-Fe-B MGs in order to achieve novel magnetic semiconductors through the metal-semiconductor transition. They mainly employed the first-principles calculations to reveal the electronic and atomic structure of Co-Fe-B-O glass. A single-phase Co-Fe-B metallic glass is discovered to transform into a Co-Fe-B-O glass. Their results demonstrate an significant step for the more comprehensive and deeper knowledge of the metal-semiconductor transition induced by oxygen doping.

Chen et al. investigated how chemical heterogeneity and grain sizes would affect Mg-Cu nano-glasses' mechanical behaviors by means of molecular dynamics simulations. They discovered that, within dual-phase nano-glass samples consisting of two distinct chemical compositions, their deformation behaviors strongly depend on the relative fraction of soft/hard phases. This is because the glass-glass interfaces are more prone to initiate the shear band formation due to more stress concentration sites at the interfaces. Their finding is critical and practical for designing new nanoglasses with the synergy of high strength and ductility.

Machine learning (ML) techniques have recently been applied in various areas of physics and material science, and promoted a better understanding of complex materials and phenomena such as mechanical deformation of MGs. Lee and Ryu employed a graph neural network model to predict initially activated deformation events in a model MG, so-called shear transformation zone (STZ), and evaluated the predictive power of the ML model using various metrics for class imbalance problem. Their findings provide a practical guide for improving ML-based prediction of the STZ atoms.

Egami and Ryu proposed a new, "*dual bottom-up and top-down approaches*" to decipher glasses' structures. They demonstrated that the competition and compromise between the local and global driving forces dictate the samples' final structures. The balance between the above driving forces can in principle be manifested by the coherence length of atomic packings measurable in experiments. These findings provide a new perspective on the distinct natures of SROs and MROs in glasses.

We believe that the Research Topic of papers in our present Research Topic not only presents some latest novel progresses in the field, but will also stimulate new exciting studies and set directions for future research in complex alloys.

Author contributions

All authors listed have made a substantial, direct, and intellectual contribution to the work and approved it for publication.

Conflict of interest

The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

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