frontiers | Frontiers in Materials

TYPE Editorial
PUBLISHED 14 December 2022
DOI 10.3389/fmats.2022.1111499

OPEN ACCESS

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SPECIALTY SECTION
This article was submitted to Computational Materials Science, a section of the journal Frontiers in Materials

RECEIVED 29 November 2022
ACCEPTED 08 December 2022
PUBLISHED 14 December 2022

CITATION
Acar P, Tran A, Nikbay M and Mahadevan S (2022), Editorial: Uncertainty quantification in characterization, modelling, and design of materials.
Front. Mater. 9:1111499.
doi: 10.3389/fmats.2022.1111499

Editorial: Uncertainty quantification in characterization, modelling, and design of materials

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KEYWORDS

uncertainty quantification (UQ), uncertainty propagation (UP), design under uncertainty, material characterization and modeling, material design, computational materials science and engineering

Editorial on the Research Topic
Uncertainty quantification (UQ) in characterization, modelling, and design of materials

Uncertainties arise from a variety of sources, including experimental/measurement errors, imperfections in manufacturing/processing, modelling and computational assumptions, lack of knowledge associated with numerical models, and model-form errors. Therefore, traditional deterministic approaches in the characterization, modelling, and design of materials often fall short of achieving trustworthy and reliable predictions of the properties and performance of materials. Several problems may occur due to the use of these traditional deterministic techniques since the uncertainty in material behaviour may cause undesirable deviations in expected material properties, which could alter the performance of structures, or even cause the failure of critical systems. As a result, characterization, modelling, and design of materials require the consideration of the influence of uncertainties on material behaviour and properties to improve the performance and reliability of structures and critical systems. Recent advances in this area include the development of theoretical, numerical, data-driven, and machine-learning-reinforced uncertainty quantification methods for applications in materials science and engineering problems across multiple length scales and time scales. This Research Topic has covered the advances in the development and application of uncertainty quantification techniques for investigating the effects of uncertainties on physical material behaviour and designing materials under uncertainty. The published studies have covered topics ranging from crystal plasticity and fatigue nucleation modelling of materials by considering the effects of material uncertainties to the

10.3389/fmats.2022.1111499

investigation of the manufacturing (processing)-induced uncertainties or experimental uncertainties with different characterization and testing techniques.

The effects of microstructural features on the fatigue nucleation life of a polycrystalline material were investigated by Zhang et al.) by utilizing uncertainty quantification techniques. For this purpose, the authors modelled random microstructural features using the Monte Carlo method. With the definition of statistical volume elements (SVEs), the effects of the microstructural uncertainty on the fatigue behaviour were analyzed . In particular, the response of each SVE under fatigue loading was predicted by the sparse dislocation density-informed eigenstrain-based reduced order homogenization model with high computational efficiency. It was further linked to the fatigue nucleation life through a fatigue indicator parameter (FIP). The presented numerical framework was validated with the fatigue response of Titanium alloy, Ti-6Al-2Sn-4Zr-2Mo .

The uncertainty arising from crystal plasticity finite element modelling of polycrystalline microstructures was quantified by (Tran et al.) using the stochastic collocation method. The uncertainty of three commonly used constitutive models, including the phenomenological models (with and without twinning), and dislocation-density-based models, was studied for three different materials: the face-centered cubic (fcc) copper (Cu), body-centered cubic (bcc) tungsten (W), and hexagonal close packing (hcp) magnesium (Mg). The authors demonstrated that the numerical results quantified the uncertainty of the constitutive models and investigated the global sensitivity of the constitutive variables .

Another important problem studied in this Research Topic is the quantification of the spatially variable mechanical response in structural materials arising from additive manufacturing by Tallman et al. . The authors investigated how these variations affect the component performance by conducting ninety-nine profilometry-based indentation plastometry tests on a traditionally manufactured Al 7075 plate sample. The resulting profilometry data and the Voce parameter predictions were analyzed to distinguish contributions of noise, individual measurement uncertainty, and additional set-wide variations .

Last but not the least, this Research Topic also covered the uncertainty propagation problem in computational materials science.James et al. presented a model for uncertainty propagation to establish confidence in numerical models and validate these models against the experiments or high-fidelity simulations which can be accepted as ground-truth information. They particularly worked on a numerical method by re-weighing the probability distributions of input parameters to enable the generation of more statistically representative samples. This method was applied to the computational modelling of materials response under high strain rates. The authors demonstrated that it could provide approximate output distributions at a lower cost compared to more traditional techniques based on the exhaustive sampling of probability distributions of random variables .

This Research Topic has provided a Research Topic of studies on uncertainty quantification and propagation in the characterization, modelling, and design of materials using different numerical strategies. However, there still remain important challenges to be addressed in this research area in the future due to the complex physics and mathematics behind the uncertainty quantification and propagation problems in materials science and engineering. These challenges relate to the current limitations arising from the lack of appropriate numerical and machine learning-driven strategies to address the aleatoric and epistemic uncertainties impacting the interplay among multiple length scales concerning processing-structure-property relationships. Additionally, the effects of the uncertainty arising from processing, experiments, and computational models need to be investigated for a wide range of different material classes such as metals, metallic alloys, composites, polymers, metamaterials, and bio-inspired systems.

Author contributions

All authors have contributed to the presented Research Topic.

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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