MULTISCALE MODELLING AND CHARACTERISATION IN STRUCTURAL MATERIALS

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ABSTRACT

This invited session focuses on scale-bridging studies using advanced computational modelling and characterisation techniques to elucidate deformation and strengthening mechanisms in structural materials. Various computational approaches, including data-driven methods [1], have been developed to bridge multiple scale levels from quantum/atomistic scales to the macroscopic scale, in an effort to better predict material responses and structural deformation behaviour. These approaches help improve our understanding of the underlying mechanisms of material behaviour, and they are also key accelerate the development of new materials with improved properties and performance. In this context, advanced characterization, including in-situ and data intensive time-resolved studies [2], are becoming increasingly important to both validate these advanced computational approaches and to discover new mechanisms. This session aims to showcase recent research using in computational, experimental, and hybrid approaches to study the behaviour of structural materials, in particular under multiple stimuli and where the structure of the materials evolves during deformation.

Topics of interest include the following:

- Scale-bridging computational approaches
- Modelling and characterisation approaches of microscopic material behaviours
- Coupling of theoretical, experimental, computational, and data-driven approaches
- Application of the above-mentioned approaches

REFERENCES

[1] Chen, T., Watanabe, I., Liu, D., Goto, K., Data-driven estimation of plastic properties of alloys using neighboring indentation test, *Science and Technology of Advanced Materials: Methods*, Vol. 1, pp.143-151, 2021.

[2] Dichtl, C., Lunt, D., Atkinson, M., Thomas, R., Plowman, A., Barzdajn, B., Sandala, R., Da Fonseca, J.Q. and Preuss, M., Slip activity during low-stress cold creep deformation in a near-α titanium alloy, *Acta Materialia*, Vol.229, 117691, 2022.