Understanding RVE-Map in the context of TiAl polycrystals for the effective analysis of structure-property relationship

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Materials discovery and development processes have been accelerated with the availability of advanced computational models and simulation tools. Yet the reliability and robustness of predictions in most discovery, improvement and design efforts are limited due to various sources of uncertainties. It is an inherent factor in various aspects of modeling, processing, design, and development of a materials-system. Model-form and parameter uncertainties are major epistemic components of error in modeling and simulation. Uncertainty is not only added from different sources but also propagated when different physics and numerics are employed to simulate different complex behaviors. One of such prime examples are scale-bridging problems where propagation of uncertainty is heavily influenced from individual scales especially when lower scale information is passed to the higher scale. So, identifying the influential sources from the lower scale can be considered as a very clever step in order to control the propagation of uncertainties. In this context, variable sizes of microstructural volume (frequently referred as RVE, or representative volume element) and their uncertainties in homogenization problems are well-known to the mechanics community [1,2]. An acceptable size is supposed to vary with the existence of different microstructural complexities (e.g. various defects like grain boundaries, lamellar boundaries, twin boundaries, anti-phase boundaries, stacking faults, dislocation network, etc.), property-contrast among different constituent phases and with the increase of different nonlinearities existing in both single and multiphysics properties (like mechanical, thermal, electrical, magnetic, thermo-mechanical, chemical, electro-mechanical, electro-magnetic etc. and so on) [2]. The reasonable size of an RVE with respect to a specific property means the behavior of the RVE is nearly independent of its boundary conditions, different realizations and larger sizes beyond optimal. For a specific property, if the considered size is too small, then the averaged property will have large uncertainties (different realizations will have largely different behaviors and different boundary conditions give different averaged responses). What would be an acceptable size for a specific property considering a specific material is not precisely known usually, until a large number of different simulations with different sizes is analyzed based on convergence study. It is also to be noted that the acceptable size is not expected to be the same for homogenized property and for local fields [1]. The fundamental assumption here is that there exists a hierarchy of acceptable-sizes of volume elements for a specific material or alloy system corresponding to different properties. This hierarchy considering phase-contrast, relative error, microstructural and property complexities has been referred here as RVE-Map. If such an RVE-Map is known then the simulation results in homogenization and multiscale problems are expected to be far more reliable. This work is the primary step toward establishing an RVE-Map.

Microstructural space for a particular materials-system can be simpler (like periodic microstructure) to very complex like random particulate microstructure, polycrystalline or randomly placed fiber-reinforced materials. Polycrystalline microstructures can be considered as one the most complex among them. A highly complex, duplex TiAl like intermetallic alloy has been chosen for this work. It is worth to mention that, if an acceptable size is very large corresponding to a complex property then finding the expected size with convergence studies would be computationally expensive and cumbersome. Machine learning techniques can play a very interesting role here in order to make faster decision by reducing the amount of computations significantly.

[1] M. Pinz *et al.*, Microstructure and property based statistically equivalent RVEs for intragranular γ−γ' microstructures of Ni-based superalloys, *Acta Materialia*, Volume 157, 2018, Pages 245-258.

[2] T. Kanit *et al.*, Determination of the size of the representative volume element for random composites: statistical and numerical approach*, International Journal of Solids and Structures*, Volume 40, Issues 13–14, 2003, Pages 3647-3679.