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Multiscale-modeling based on molecular-dynamics and phase-field approaches: Growth kinetics in pure Fe and binary alloy NiZr

M Guerdane
Karlsruhe Institute of Technology, Germany

One of the central challenges in multiscale modeling consists of how to bridge the gap among atomistic and macroscopic approaches in order to ensure that the descriptions at all levels are quantitatively consistent with each other. In our work, we carry out this task for the hierarchical coupling approach that combines molecular dynamics (MD) with phase-field (PF) modeling. The consistency analysis is achieved by detailed comparisons of quantitative predictions of the considered modeling methods for the growth kinetics. The latter is a typical multiscale problem in material physics. The MD simulations provide the physical quantities needed for the construction of the multiscale models. Of central importance are the bulk free energy and the solid-liquid interfacial free energy. We consider the monatomic system Fe and the binary alloy NiZr. We discuss in particular the solid-liquid interface diffusion, the interfacial thickness anisotropy, and their determining influence on the growth kinetics.

mohammed.guerdane@kit.edu

Development of new Spark Plasma Sintered (SPS) composite materials reinforced with single crystal alumina fibers (NKR®)

Víctor Valcárcel
Neoker S L, Spain

High performance advanced composites are mainly used in structural applications, where the main concerns are mechanical performance (stiffness, strength, creep and fatigue resistance), although many other properties can dominate the selection procedure (electrical conductivity, thermal conductivity, dielectric properties, etc.). The most suitable variant has to be chosen on the basis of this application-driven "wish list". Of course, the final properties of a composite will always be determined both by their composition (the matrix and the reinforcing phase) and by their fabrication procedure. When a novel material is employed as a reinforcing phase, conventional fabrication routes will often offer limited possibilities and limited performance, and therefore disruptive sintering strategies are needed to achieve the best potential from such a new composite. The novel single crystal alumina fibers, produced by Neoker, possess a huge potential to be used as a reinforcing phase in high performance composite materials. As an oxide, alumina can offer chemical stability where non-oxides (carbon, carbides, nitrides etc.) are likely to fail. As single crystals, they are defect-free, and as fibers, NKR® big aspect ratio (length/diameter) allows a big increase in the mechanical performance of the composite compared to the bulk material. Here we are presenting our preliminary results, where we have demonstrated that Spark Plasma Sintering is able to overcome the main difficulties of incorporating NKR® fibers in composites, so it can be considered one of the most promising sintering routes for this new family of materials. In this work, different matrix compositions have been combined with different NKR® fiber percentages using SPS route. The use of different coatings has been explored, trying to improve the matrix-fiber interface, thus activating fiber strengthening. Most relevant features of the final composite have been analyzed, focused on density, porosity and mechanical performance (bending strength, toughness etc.). In this work, we have been able to demonstrate that NKR® fibers combined with the SPS route gave rise to composite materials with high densities and homogeneous microstructures, allowing good control of interface properties, and therefore achieving high mechanical performances. This combination of NKR® fibers and SPS route will bring unique opportunities to create new high added value composite materials.

valcarcel@neoker.org