

A roadmap for the virtual design of metallic materials: From atoms to components



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A simulation roadmap is presented to carry out virtual design, virtual processing and virtual testing of metallic alloys for engineering applications. The strategy is based on a bottom-up, multiscale modelling approach which runs along two parallel lines: simulation of the microstructural development during processing (virtual processing) and simulation of the mechanical behavior from the microstructure (virtual testing). Modeling efforts begin with ab initio simulations and bridging of the length and time scales is accomplished through different strategies which encompass the whole range of length and time scales required by virtual design, virtual processing and virtual testing. Nevertheless, not everything can or should be computed and critical experiments are an integral part of the strategy for the calibration and validation of the multiscale strategies at different length scales. Two examples of application of the different parts of the strategy for virtual processing and virtual testing are presented in detail.

Prof. Javier Llorca is scientific director and founder of the IMDEA Materials Institute and professor and head of the research group on "Advanced Structural Materials and Nanomaterials" at the Technical University of Madrid. He got his PhD in Materials Science from the Technical University of Madrid and has held visiting appointments at Brown University, Shanghai Jiao Tong University and Indian Institute of Science. Prof. Llorca, a Fulbright scholar, is Fellow of the European Mechanics Society and member of the *Academia Europaea* and has received the Research Award from the Spanish Royal Academy of Sciences.

His research activities have been focused in the systematic application of computational tools and multiscale modeling strategies to establish the link between processing, microstructure and properties of structural materials. A key feature of his contributions is the use of novel experimental techniques to determine the properties of the phases and interfaces in the material at the nm and μm scale. So, simulations are fed with experimental values independently obtained and free of "adjusting" parameters. Some of these developments have become the foundation of the modern techniques of virtual testing of composites, which are starting to be used by the aerospace industry to minimize the number of costly mechanical tests to characterize and certify composite structures.

His current research interests –supported by an Advanced Grant from the European Research Council– are focused in the development of multiscale modeling strategies to carry out virtual design, virtual processing and virtual testing of metallic materials, including the experimental validation at different length scales, so new alloys can be designed, tested and optimized *in silico* before they are actually manufactured in the laboratory.

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