

Computational Steel Design – Chances and Limits of Materials Modelling

Wolfgang Bleck and Ulrich Prahl

Department of Ferrous Metallurgy, RWTH Aachen University

Email: bleck@iehk.rwth-aachen.de

ulrich.prahl@iehk.rwth-aachen.de

Any production is based on materials eventually becoming components of a final product. Material properties thus are of utmost importance both for productivity and reliability of processing during production and for application and reliability of the product components. A sound prediction of materials properties thus is highly important. Such a prediction requires tracking of microstructure and properties evolution along the entire component life-cycle starting from a homogeneous, isotropic and stress-free melt and eventually ending in failure under operational load.

In almost all nature and engineering scientific disciplines the computer simulation reaches the status of an individual scientific method. Material science and engineering joins this trend which permits computational material and process design increasingly. The aim of this contribution is to give an exemplary overview on current trends in virtual material development and to show the next development steps.

Ongoing activities at the RWTH Aachen University will be presented. For knowledge driven design of materials and processes two topics will be addressed: First, the establishment of a virtual platform for materials processing comprises a virtual, integrative numerical description of processes and of the microstructure evolution along the entire production chain. Secondly, the development of ab initio methods promises robust predictability of properties based on chemical composition.