Multiscale Simulation of Metals from Atoms to Components

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Abstract

In this overview it will be shown how the first successful example of real multiscaling for metals was achieved.

Multiscale simulation in the present context means the involvement of all length scales from atomistics to micromechanical contributions up to macroscopic material behavior and further up to applications for components.

The main focus of the presentation will be put on the methods involved and how they interact within the present approach. It will be shown that each method is superior on the respective length scale. Furthermore, the parameters which transport the relevant information from one length scale to the next one are decisive for the success of physically based multiscale simulations.

While in the past different methods were tried to be combined into one simulation it is nowadays obvious in many fields of research that the only way to succeed in understanding the mechanical behavior of materials is to do sequential multiscale simulations in order to achieve physically based practical material solutions without adjustment to any experiment.

In a final step it will be shown that the approach is not limited to metals but can be extended to nearly arbitrary material classes and even for composites as well as any aspect of material problems in modern technical applications where all disciplines meet, from physics to material science and further on to engineering applications.

References

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