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PHYSICAL MULTISCALE FATIGUE MODELING FROM ATOMS TO COMPONENTS WITHOUT EXPERIMENTS

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In this overview the first successful examples of real multiscaling from atoms to macroscale for different applications for metals are presented. Multiscale simulation comprises all length scales from electrons/atoms via micromechanical contributions to macroscopic materials behavior and further up to applications for components, frequently called multiscale materials modelling (MMM) (Fig. 1).

A main focus of the presentation will be put on new developments with special emphasis on MD-simulations and other 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 performing physically based multiscale simulations [1,2].

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 apply scale bridging techniques in sequential multiscale simulations (Fig. 2) to achieve physically based practical material solutions without adjustment to any experiment. This has opened the door to real virtual materials design strategies.

In a final step it will be shown that the approach is not limited to metals but can be extended to other material classes and can be also applied for composites [3] as well as to many aspects of material problems in modern technical applications where all disciplines meet, from physics to materials science and further on to engineering applications. Emphasis will be put on the problem of fatigue of metals where multiscale materials modelling can provide the answer to numerous questions such as the influence of the lattice type or the relevance of materials properties. A new rule for fatigue strength is derived based on the critical resolved shear stress (CRSS).

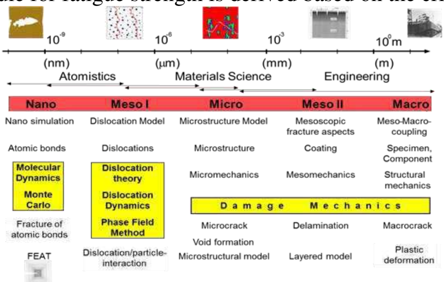

Fig. 1. Multiscale Materials Modelling (MMM)

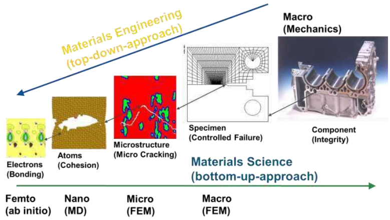

Fig. 2. Scale Bridging Technique

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