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Interrupted by stays at the National Institute for Materials Science in 2017 (Tsukuba, Japan 2017) and at the University of California, Los, Angeles (2019) he continued his academic career at the Max-Planck-Institut für Eisenforschung - First as postdoctoral fellow (2015-2019) and then as group leader for Integrated Computational Materials Engineering (2019-2020).

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Crystal Plasticity Simulations of Complex Microstructures

The potential of metallic materials such as steel and copper - although they have been used by mankind for thousands of years - is far from being exhausted. Nowadays, computer simulations help to find the ideal material for the manufacturing of engineering parts such as car bodies, bridges, or turbine blades.

Metallic materials that are used in automotive, aerospace, and civil engineering consist of a large number of individual crystals. These crystals are arranged in a space-filling manner - comparable to bubbles in a foam – and differ in their shape and size. The crystals themselves consist of regularly arranged atoms. Due to its atomic structure, crystals have a anisotropic mechanical behavior, i.e. the force that is required to deform a crystal depends on its orientation relative to the crystal structure. A metal behaves isotropic only if it consists of many individual crystals and if the orientation of these crystals is randomly distributed. In order to assess existing materials or to develop improved materials, it is therefore of great importance to understand the interactions between the crystals when the material is deformed. After all, it is the common behavior of all crystals under the influence of their neighborhood that determines the material behavior.

If one bends a metallic material large enough, the deformation is only partially recovered after the force is removed. This makes it possible to use metals as springs and at the same time manufacture a car chassis through targeted deformation from flat sheet metal. Both the elastic (reversible) and the plastic (permanent) part of the deformation are direction-dependent in the individual crystal. Elastic behavior occurs when the individual atoms are shifted from their regular arrangement relative to one another without changing their neighborhood relationships. The plastic behavior, on the other hand, is mainly based on the movement of dislocations. Dislocations are a disorder in the regular crystal structure. While dislocations enable the plastic deformation of metals, they also hinder the movement of other dislocations in the crystal and thus make further deformation more difficult. This behavior, known as hardening, can be observed, for example, when bending a paper clip. The exact description of the complex interactions of dislocations is the subject of current research in the field of crystal plasticity.

Based on the microstructure, i.e. the description of the crystal geometry and orientation, the behavior of a material can be calculated on the computer. A typical calculation consists of 50–1000 individual crystals, which are arranged next to each other to fill space and are crushed together. Each crystal is in turn represented by up to 10,000 similarly oriented voxels, whereby a voxel is the extension of a pixel, as used in digital image processing, to three dimensions. The behavior of all atoms in a voxel is described by the elastic-plastic model presented above, which means in particular that the atoms do not have to be described

individually. This enormously shortens the computation time. The quality of the calculation therefore depends on whether the common behavior of the atoms - and in particular their plastic behavior - is correctly described by the model used. If a microstructure is crushed, the individual crystals deform differently depending on their orientation in such a way that overall the least amount of force is required. A fast and precise mathematical method is required to efficiently calculate this physically possible state in the model. The so-called spectral method is especially suited for this problem. This elegant mathematical formulation makes it possible to calculate the behavior of microstructures - which are representative of the examined material - with unprecedented accuracy and in shot time. Another big advantage of the spectral method, besides its speed, is the simple use of experimentally determined microstructures as a basis for calculations. In cooperation with experts for the experimental investigation of materials, I was able to compare the results of my calculations directly with experimentally determined data. The comparison has shown that the approach I used and presented here is able to correctly reproduce the experimentally observed material behavior. This makes it possible to replace time-consuming and expensive tests on real materials with inexpensive and fast computer calculations.

Micro-mechanical simulations are especially important for complex materials such as dual-phase steels. These steels consist of a comparatively ductile matrix made of ferrite which is reinforced with solid but brittle martensite. The mechanical behavior of a dual-phase steel therefore depends on the anisotropic properties of the two phases as well as the volume fraction and distribution of the martensite. An example of such a simulation is shown in Fig. 1.

The interdisciplinary approach, in which methods from mathematics, computer science and physics are combined, allows the description of processes on the atomic level to be transferred to the behavior of entire components. The computer calculations make it possible to understand and improve the behavior of metallic materials. With these improved materials, more energy-efficient - because lighter - cars and airplanes and safe high-rise buildings can be built.

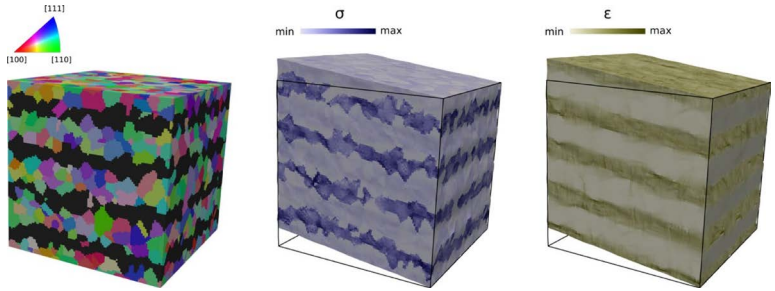

Figure 1. Crystal plasticity simulation of a dual-phase steel: Left: Undeformed microstructure, the ferritic grains are collored according to their crystallographic orientation (inverse pole figure, IPF) and the martensitic phase is shown in black. Middle: equivalent stress at approx. 10% shear deformation. Right: Equivalent strain at approx. 10% shear deformation