A New Finite Element Method for Predicting Anisotropy of Steels

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Scientists from the theory group in the Department for Microstructure Physics and Metal Forming at the Max-Planck-Institut für Eisenforschung in Düsseldorf in Germany have developed a new finite element method for the prediction of elastic–plastic anisotropy during steel forming. The novelty of the approach consists in merging formerly separated concepts from metal physics, crystallography, and variational mathematics. The method is referred to as texture component crystal plasticity finite element method (TCCP-FEM). The new approach is based on the direct integration of a small set of spherical crystallographic orientation components into a non-linear finite element model. It allows for the first time to integrate fundamental theory from the fields of crystallography and crystal plasticity into the theoretical treatment of the microscopic and macroscopic behavior of steels at reasonable computation times. The method is hence particularly suited in industrial context for instance for predicting the mechanical properties of novel steels for light-weight constructions.
We encounter metals typically in the form of polycrystalline aggregates where each crystal, also referred to as grain, can have a different orientation of its crystallographic axes with respect to the external reference system. The distribution of these orientations is referred to as texture. The discrete nature of crystallographic atomic-scale shear along densely packed lattice directions on preferred crystal planes entails a highly anisotropic (orientation dependent) response of such aggregates during mechanical loading. This applies in particular for polycrystalline steels, where the grains interact with their neighbor crystals during forming and continuously change their crystal orientation.

Research on large strain plastic anisotropy of metals has been a topic for more than 4000 years. The reasons are obvious: Engineers want to save material, obtain similar mechanical properties everywhere in the material, and avoid failure. The computational treatment of crystal anisotropy requires close integration of approaches from metal physics, crystallography and mathematics of non-linear differential equations.

While the elastic-plastic deformation of a single crystal as a function of its orientation can nowadays be well predicted, plasticity of polycrystalline steels is less well tractable. This is essentially due to two reasons. First, the intricate elastic-plastic interaction occurring during co-deformation among the highly anisotropic individual grains and their respective neighbor crystals as well as among different regions within the same grain are not well understood. Second, crystals gradually change their orientation during forming and hence also alter the overall anisotropy of the entire specimen. The described processes entail strong heterogeneity in mechanically loaded crystalline matter in terms of strain, stress, and crystal orientation. Well known consequences of this behavior is for instance the elastic spring-back effect in automotive sheet forming production lines.

Besides fundamental questions from the field of polycrystal mechanics also engineering
problems would considerably profit from novel theoretical approaches. Research on elastic-plastic anisotropy is a topic of high economic relevance since improved predictions of forming operations can help saving raw material, obtaining similar mechanical properties everywhere in a formed product, avoiding failure, and optimizing forming of light-weight constructional steels.

The computational treatment of crystal anisotropy requires close integration of approaches from metal physics, crystallography and mathematics of non-linear differential equations. The major challenge of the present initiative at the Max-Planck-Institut to directly integrate physically based crystal behavior into variational approaches lies in identifying an effective method of mapping a representative crystallographic orientation distribution on the integration points of a finite element method using a compact mathematical form which permits texture update during mechanical loading.

Example of a simulated large strain forming operation including crystallographic orientation information and rotation of the crystals during straining. The importance of the crystallographic texture can be seen from the resulting shape revealing the so called earing phenomenon. The simulations are elastic-plastic, i.e. spring back prediction is automatically included. The gray scale scheme indicates von Mises strains.

Based on these fundamental considerations Max-Planck researchers have now developed a new physically based and highly time efficient prediction method for the simulation of polycrystal elasticity and plasticity which accounts for all relevant crystallographic aspects. Its idea is to map a discrete representation of an orientation distribution onto each integration point of a non-linear crystal plasticity finite element formulation. When taking a practical perspective it is obvious that an appropriate representation of a discrete texture requires the reduction of the information content to a level at which complex mechanical loading situations can be simulated without the help of a supercomputer. Hence, a texture reproduction method was chosen which is based on using discrete spherical Gauss functions.
This approach provides a very small set of orientational components which are characterized by simple parameters of physical significance (Euler angle triple, volume fraction, full width at half maximum). Using this method, only a few texture components are needed to describe the orientation distribution function. This data reduction increases computing efficiency dramatically. The required orientation components can be extracted from experimental data, such as pole figures stemming from x-ray, neutron-, or electron diffraction.

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