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Advanced Deformation Process Modeling

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Abstract

This is the final report of a three-year, Laboratory Directed Research and Development (LDRD) project at the Los Alamos National Laboratory (LANL). Significant progress was made in achieving a comprehensive and coherent description of material behavior in deformation processing. The materials included were metals, alloys, intermetallic compounds, arbitrary lattice structure, and metal matrix composites. The aspects of behavior modeled include the kinetics of flow and strain hardening, as well as recrystallization and the various anisotropies of strength and compliance. Highlights include a new prediction of the limiting strength of materials at high temperature, a new understanding of the generation of new grain boundaries during forming operations, and a quantitatively verified computer simulation of texture development and the resulting behavioral anisotropies.

Background and Research Objectives

An extensive base of fundamental knowledge has been accumulated over the last four decades concerning the microscopic mechanisms and phenomenological laws that explain or describe various aspects of plasticity. Integrating these individual components of understanding into a complete and coherent description of material behavior has only been worked on for a few years, by a few people, and is not as yet definitive. This lack of attention to general, overall macroscopic behavior on the part of materials scientists is perhaps the reason why the rules for material response used in even the most sophisticated

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engineering codes today have remained at the materials science level of the 1950s, with the exception of some recent efforts between Los Alamos scientists and their collaborators.

Similarly, for approximately three decades, textures in materials have been researched intensively from fundamental and empirical points of view. However, to this day textures are not routinely measured for the purpose of their main macroscopic effect: the anisotropy of materials properties, which can be substantial indeed. The primary reason for this omission has been the nonexistence or awkwardness of methods to analyze measured textures in a useful way and to use this information for quantitative predictions of macroscopic properties, except for the one developed over the last few years at Los Alamos.

This project's aim is to integrate these components of understanding into a comprehensive, coherent description of material behavior in deformation processing. The product that was aimed for does not only consist of rules and equations, but also includes useful subroutines for macroscopic computer codes, prescriptions for determining the parameters required for applications of the model, and diagnostic techniques for ascertaining its applicability in a particular application. Materials included metals, alloys, and intermetallic compounds.

Importance to LANL's Science and Technology Base and National R&D Needs

This project's significance is that it has been actually implemented in a new computer code to treat complex boundary value problems. This work has been done in collaboration with a researcher at an industrial enterprise (Reynolds Metals), where the major interest is deformation processing. The code under development makes use of massively parallel programming from the ground up. It may eventually become a new standard of excellence for finite-element codes in which accurate descriptions of plasticity are crucial. A scientific byproduct of this integration of materials descriptions with boundary-value solvers is the inverse application: to scrutinize mesoscopic materials behavior by using finite-element modeling (such as the development of potential recrystallization nuclei during plastic deformation of polycrystals).

An integration with experiments is also crucial. This takes place at three levels. First, detailed prescriptions will be developed to determine the materials parameters appropriate for the model. Second, the model must be verified in a regime that is predicted to hold but is beyond the reach of easy measurements. And third, a number of examples of

actual forming processes of a well-characterized material must be undertaken in parallel with the modeling of the same process with all the actual variables as input.

The Laboratory is a world leader in making large computing facilities useful. Our code was developed for the CM-5 and, in turn, helped in developing computational strategies for parallel computers. It is now imperative to make the code portable to other mainframes and workstations. The Laboratory's Computational Test Bed is expected to help in sharing our progress in a tangible manner with other investigators and engineers, and thus foster industrial competitiveness. There is considerable expertise at the Laboratory with respect to large engineering design codes in which materials properties traditionally have been treated with little benefit from modern materials science understanding. After demonstrating our capability to integrate modern materials descriptions into our own engineering code, these material descriptions also could be implemented in the Laboratory's major traditional engineering codes.

Scientific Approach and Accomplishments

Anisotropic behavior has been shown as too complex and varied to be represented in the form of equations: numerical schemes are necessary to achieve the required degree of accuracy. A rather general numerical simulation method, in the Los Alamos polycrystal plasticity (LApp) code, has been established and implemented for cubic and hexagonal metals under multi-axial straining conditions. This code has been made available on PCs—thousands of grains can be run in minutes. At the other extreme, Paul Dawson ran 256 grains at 1500 nodes in a finite-element code on a Connection Machine. A prediction and comparison with simultaneous experiments of the developing strain heterogeneities during hydroforming have been successful and were executed in an overnight run on CM-2. Anisotropies predicated on the basis of initial and developing textures should be much more representative of material behavior than either current phenomenological assumptions or the few possible measurements could provide.

Problems in which an understanding of the material behavior itself requires (or is certainly substantially aided by) large finite-element calculations are those involving mesoscopically heterogeneous deformation. An extreme case that already has been treated is that of plasticity in metal-matrix composites. A more subtle case concerns the heterogeneities that develop near grain edges as a consequence of plastic deformation. They have never been treated in any detail and are deemed unimportant for plasticity itself; however, they may be instrumental in developing nuclei for static or dynamic

recrystallization and thus may control the behavior. To date, no macroscopically useful constitutive relation is known.

For all these applications, the initial texture of the material must be known; it is rarely random. The evaluation and representation of texture measurements, as well their use as input for predictions of polycrystal anisotropies, require attention to many details that have been worked out and condensed into a comprehensive software package ("popLA: preferred orientation package—Los Alamos"). As applications extend, new problems arise that need to be fixed or added. Pure and solution-treated metals and minerals of cubic, hexagonal, trigonal, and orthorhombic crystal symmetry and arbitrary sample symmetry can now be described. This package is used widely by government and industrial laboratories, as well as universities, from whom we occasionally get useful feedback. The maintenance of this code will continue to require some attention.

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