steady, laminar process. This is because reconnection could well be a very turbulent process—both in time (intermittent) and space (patchy). Moreover, the effects of boundary conditions need to be more realistically taken into account. The desired resolution to these issues will be driven by more advanced diagnostic and computational approaches which will enable progress in uncovering the interrelationship between local plasma dynamics in the reconnection layer and global boundary conditions.

Even as the debates continue on the Sweet-Parker model versus the Petschek model, on the nature and cause of anomalous resistivity, and on the relationship between magnetic reconnection and dynamo mechanisms, the emergence of ways to study these issues provides hope for substantive breakthroughs. After the workshop, Petschek commented that "I found the meeting very stimulating. In particular, I had not been aware of the number of ways people have found to calculate reconnection rates. The new experiments are very nice. If one has been looking at interpretations based on single satellite measurements, the rakes of magnetometers (the internal probes on MRX) seem to generate huge amounts of correlated data which makes interpretation so much easier."

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MATERIALS SCIENCE

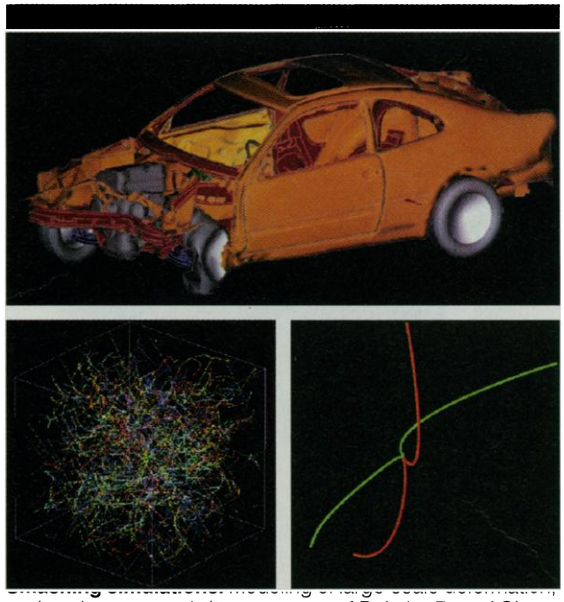
A Dislocation Crash Test

Peter Gumbsch

What makes an atomic-level simulation of lattice defects in pure copper crashing into each other interesting? Not the detailed results of the multimillion-atom calculation reported by Zhou *et al.* on page 1525 of this issue (*1*), but rather the idea that such simulations can contribute one important missing part of a big puzzle: the physical basis for the engineering description of the deformation of materials.

For engineering simulations of a car crash (see figure, top) or of metal-forming processes such as deep drawing or rolling, continuum mechanical techniques like the finite element method are exclusively used. Any such continuum description requires the specification of the governing constitutive equations, that is, equations that relate the response of a material to an applied force. Currently, the necessary parameters are empirically adjusted to experiments, but simulations could in the near future allow these constitutive equations to be determined from physically based simulations.

Materials deformation consists of a well understood elastic contribution and a permanent plastic contribution. The plastic deformation is mainly carried by dislocations, line-defects of the regular crystal lattice. When a dislocation moves through the crystal, it shears the crystal along its plane of motion (slip) by a well-defined displacement vector. Different dislocations strongly interact with each other (*2*). The long-range interaction can be well described by linear elasticity theory, which is sufficient for many applications of dislocation mechanics. The short-range interaction, however, is crucial when one dislocation intersects another or changes its slip plane (cross-slip). In order to simulate large macroscopic deformations, it is necessary to consider many dislocations and all of their interactions and their dynamics.



such as in a car crash (**top**, courtesy of Daimler-Benz AG), requires equations that describe the response of a material to an applied load. In the near future, one may be able to obtain such equations from discrete dislocation simulations (**bottom, left**, courtesy of B. Devincre CNRS/ONERA); these, in turn, require atomistic input on dislocation core structure, cross slip, and dislocation intersection (**bottom, right**).

Six years ago, a French research group (*3*) first simulated such dislocation motion on the basis of interacting discrete, straight dislocation segments in its full three-dimensional complexity (see lower part of figure) and has since led the field. These discrete dislocation dynamic (DDD) simulations serve two main purposes: First, they help us understand the processes that lead to self-organization and structuring of the dislocation fields, and second, they have the potential to give a physically based description of the materials' response during deformation, which can then be used for continuum modeling (*4*).

The DDD simulations need to be given mobility laws, which describe how a dislocation responds to a stress acting on it. Although one generally has to consider the whole dislocation structure, in some metals and in certain temperature regimes, this response critically depends only on one individual dislocation type. An example is the low-temperature deformation of body-centered cubic metals like iron or molybdenum, where the screw dislocation is known to control the plastic response (*5*). Its properties can reasonably well be understood in qualitative terms by analyzing the core of the dislocation atomistically (*6*). Such atomistic studies of the core structure

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of individual dislocations have been possible for almost 30 years, albeit in a rather crude manner owing to the lack of refinement of the interatomic potentials. It is only recently that atomistic studies reached a sufficient level of sophistication to really start becoming quantitative.

Similarly, until a few years ago, it was simply impossible to study the other atomistic aspects of dislocation mechanics, namely, cross-slip and dislocation intersection. Both processes have now been tackled. Last year, an elegant atomistic modeling technique was applied to model cross-slip in copper (*7*). More recently, Zhou *et al.*, in this issue (*1*), and Bulatov *et al.* (*8*) have presented studies of dislocation intersections. These atomistic simulations encompass millions of atoms and generate such a vast amount of information (some 10^4 configurations of 10^6 atoms) that one of the most important steps is to discard most of it, namely, all the atomistic information not directly connected to the cores of the dislocations. What is left is a physical picture of the atomic configurations in such a dislocation intersection and even some quantitative information about the stresses required to break the junction.

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This atomistic study focuses on one of many different dislocation intersections in only one particular material, pure copper. Nevertheless, it exemplifies where atomistic modeling could in the near future contribute to the understanding of the mechanics of materials. Properly quantified, the atomistic simulations may contribute the last missing bits of information for the direct DDD simulation of macroscopic deformations based exclusively on physically transparent "rules." Such a comparison would mean directly calculating, as compared to empirically adjusting, the governing constitutive equations of continuum mechanical models of the deformation of materials.

Atomistic simulations still have a long way to go if they are to capture the full complexity of the dislocation core mechanisms contributing to the mechanical behavior of model materials, not to mention more complicated alloys. However, the present developments hold great promise that a link can eventually be achieved between atomic scale and macroscopic large-scale deformation.

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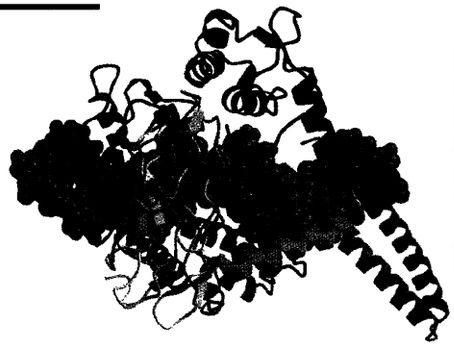
PROTEIN STRUCTURE

Topological Nuts and Bolts

Howard A. Nash

Most enzymes do chemistry—catalyzing reactions that change the covalent structure of a substrate. But with some enzymes that work on polymeric substrates, the end result is a mechanical rather than chemical change. Among these are the topoisomerases, which can untwist superhelically coiled DNA. Starting with the first example some 25 years ago (*1*), these enzymes that can change the topology of DNA have been the subject of elegant mechanistic and biological studies (*2*). On pages 1504 and 1534 of this issue, we get a first but very informative look at the structure of human topoisomerase I (*3*, *4*), whose importance is highlighted by its identity as the target of an important class of anticancer drug.

In a molecule of DNA without free ends, the number of times two polynucleotide strands wind around each other is fixed. This topological invariance is the inevitable consequence of the continuous DNA backbone, which forbids the two chains to pass through one another. Accordingly, an enzyme that alters DNA topology must break at least one strand. And, to restore the physical continuity of the DNA after the ensuing change in interwinding, the enzyme must also seal the break. Exactly as predicted in the initial study (*1*), this reversible breakage is achieved because topoisomerases maintain the high-energy status of the phosphodiester bond during unwinding. Nucleases, another class of DNA-cleaving enzymes, hydrolyze a phosphodiester in the backbone of DNA to a phosphomonoester. In contrast, topoisomerases use an enzyme residue (typically a tyrosine) to break DNA. A new enzyme-DNA phosphodiester is formed in the process. Since the new bond is of comparable energy to the original phosphodiester, the covalent DNA-enzyme intermediate can be readily attacked by the previously liberated end of DNA to restore free enzyme and produce intact, rejoined DNA.



REDINBO, STEWART, CHAMPOUX, AND HOL

Topoisomerase I ready to unwind DNA. The intact DNA strand is in cyan, and the strand transiently nicked by the enzyme as part of the relaxation event is in magenta and pink. The polypeptide backbone of the catalytic core of the protein is shown as a ribbon.

Reversible cleavage is an artifice that has arisen in nature more than once. In eukaryotes there are at least three major types of topoisomerases—nonhomologous enzymes that are distinguished biochemically by the number of strands cleaved and whether the liberated end comes from the 3′ or 5′ side of the phosphodiester (*2*). All three are important: Disruption of any one is either frankly lethal or causes substantial defects in DNA metabolism. Topoisomerases appear to be especially important in growing cells, presumably to deal with the topological complexities arising from replication, and several potent anticancer therapies achieve their effects by pharmacological inhibition of either topoisomerase I or II (*5*).

Scientists have been fascinated with the detailed mechanism of these enzymes. Not only is phosphodiester catalysis of interest in itself, topoisomerases somehow let DNA strands change their interwinding. In doing this, the enzyme must permit (or even encourage) the transiently unshackled strands to move with respect to each other, but not so far as to preclude subsequent rejoining. In recent years, structural information has become available for two of the topoisomerase families (*6*, *7*); the present work completes the picture.

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