bacteria (*4*, *6*) have something else in common with Sun *et al*.'s microbe (*3*)—they can produce energy for growth only through dehalorespiration. So, how did these bacteria survive before (roughly) 1950, when chlorinated solvents largely replaced supposedly "harmful" hydrocarbon solvents as cleaners and degreasers? We simply don't know.

Isolation of new bacteria is the first step in developing an understanding of how subsurface bioremediation works. Studying the degradation enzymes of these microbes and their regulation—as well as genetic relationships among all subsurface microorganisms—will provide new insights into bioremediation. For example, it should reveal how degrading organisms arose within contaminated environments; what regulates expression of degradation abilities; how those abilities can be enhanced in situ; how bioremediation can be modeled; and how to predict whether intervention is required (enhanced bioremediation) or whether remediation will be adequately protective if the site is left alone (monitored natural attenuation). Finally, bacterial isolates can be used to develop molecular probes for detecting the presence of specific organisms and expression of their degradation enzymes.

Unfortunately, only a small fraction of microbes can be cultured in the laboratory. This failure may reflect unsuitable conditions, or the complex but obligative interdependence of coinhabiting species in soil. The search for new contaminant-degrading bacteria now sometimes *begins* with a molecular fishing expedition: Genetic material is extracted from contaminated sites and analyzed to see which categories (guilds) of organisms are present. If the fisherman is fortunate (see the figure), this expedition results in the isolation of new microbes based on the hints provided by molecular biology. Even if a new microbe cannot be isolated, molecular techniques allow the study of bioremediation in mixed microbial cultures. Indeed, it is now possible to probe for and study enzymes without ever isolating the organisms that produce them.

The Sun *et al*. report is the latest entry in our catalogue of contaminant-degrading microbes and their enzymes. Where is this science headed? In the not-too-distant future, it should be possible to use array-based probes containing thousands of markers to detect potentially important contaminant-degrading bacteria, the bacteria that aid them or compete with them, and to determine whether they express degradation enzymes. Armed with such information, scientists and engineers will be able to make informed decisions about remedial options, leading to less-expensive site-characterization and more-reliable bioremediation. Good fishing!

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PERSPECTIVES: MATERIALS SCIENCE

A Synchrotron Look at Steel

Matthias Militzer

On page 1003 of this issue, Offerman *et al*. describe a highly original experimental approach to studying phase transformations in steels (*1*). The method should play a key role in understanding and improving high-strength steels.

Steel is used far more extensively than any other metal or alloy as a structural material. Although it may be considered a traditional material, new steel technologies frequently enable new or improved products in a broad range of industries. Consider for example the development of novel sheet steels, driven primarily by the demands of car manufacturers. The weight fraction of steel and iron in an average family car has decreased from 74% in 1978 to 67% in 1997. Yet over the same time period, that of high-strength steels has risen from 4% to 9% (*2*). This increase is the largest growth of any material class in automotive applications and is far higher than that of other lightweight materials such as aluminum, magnesium, plastics, and composites.

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Manufacturers around the world face further challenges to increase the fuel efficiency of automobiles while improving safety and performance and maintaining affordability. The steel industry has responded to these challenges by developing advanced high-strength steels with low carbon content (below 0.2% by weight). The superior properties of these steels will permit significant vehicle weight savings, thereby reducing fuel consumption (*3, 4*).

These novel steels are multiphase steels such as dual-phase and transformation-induced plasticity (TRIP) steels, which combine high strength with excellent formability (see the figure). A recent study projected dual-phase steels to become a key component (74% by weight of the proposed vehicle body structure) in new automobile designs (*4*). Thus, a worldwide research effort is devoted to developing new generations of multiphase steels (*3, 5, 6*).

All low-carbon steels undergo processing steps, such as hot rolling, at temperatures where the face-centered cubic crystal phase (known as austenite) is stable. During subsequent processing (for example, cooling) the high temperature–phase austenite decomposes into a body-centered cubic phase (ferrite). Depending on steel chemistry and processing conditions, other more complex nonequilibrium structures such as
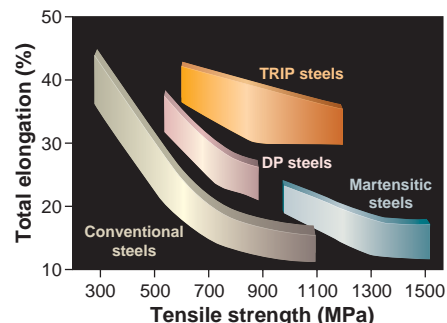
Ductility-strength relationship of steels. As tensile strength increases, conventional steels show a decrease in elongation to failure, which is a measure of formability; that is, the higher its strength, the less formable is the steel. Dual-phase (DP) and TRIP steels deviate from this general rule by combining high strength with significantly higher elongation values than those of conventional steels of the same strength level.

pearlite, bainite, or martensite may also form. The properties of steel depend critically on the microstructure obtained as a result of austenite decomposition. By tightly controlling this phase transformation, steels can be produced with multiphase microstructures and the associated superior properties. For example, dual-phase steels are essentially a composite material where a hard phase (martensite) is embedded in a soft phase (ferrite).

A detailed knowledge of the austenite decomposition kinetics in iron and steel is therefore of critical importance to the development of new steel grades and the design or optimization of industrial processing routes to consistently produce high-quality

steels. Knowledge-based process models take the microstructure evolution into account explicitly. These models are gaining increasing attention as a predictive tool that allows the operational parameters of an industrial process to be linked quantitatively with the properties of the steel product. Current austenite decomposition models with predictive capabilities for industrial conditions are empirical or semi-empirical in nature (7) and there is a need to develop fundamental model approaches.

Phase transformations in steels have been investigated more extensively than those in any other material. Any phase transformation involves two stages: nucleation and growth. The austenite decomposition usually follows a sequential pattern. In low-carbon steels, it starts with the formation of ferrite, followed by the formation of other transformation products including pearlite, bainite, and martensite (7, 8). However, the mechanisms of the entire transformation process are not fully understood. For example, the role of alloying elements (such as Mn, Mo, Si, Cr, and Al) is poorly understood.

Further understanding of the transformation mechanisms depends critically on the available characterization techniques. Classical phase transformation studies in steels measure changes in specimen di-

mension to record the volume change associated with the austenite decomposition (9). The resulting microstructures are usually observed in an optical microscope. Electron microscopy can be used to increase resolution to the nanometer range. However, the investigated area becomes so small that it limits the statistical relevance of the observations. A number of other techniques can be used to study phase transformations in steel, including neutron and x-ray diffraction, magnetic, and ultrasonic measurements.

Offerman et al. have developed an innovative technique to investigate phase transformation in situ with x-ray diffraction at a synchrotron source. By obtaining information on the nucleation and growth of individual ferrite grains in the bulk of the steel specimen, the authors provide new insights into nucleation and growth mechanisms. Extending the limited nucleation data from earlier microscopy studies (10, 11), the authors reach new conclusions on the activation energy of ferrite nucleation. Further, the results confirm classical diffusional growth for a majority of grains, but also indicate more complex growth regimes.

Experimental observations with state-of-the-art techniques, such as that presented by Offerman et al., are crucial for the develop-

ment of fundamental phase transformation models. Better understanding of phase transformation in steels should in turn help to better control these transformations and develop steels with superior properties.

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Molecular "Ghosts"

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The tremendous utility of porous materials such as zeolites (1) in catalysis and separation science has led many solid-state chemists to believe that nonporous equals noninteresting. Pores and channels dramatically increase the effective surface area of a solid, facilitate molecular diffusion, and provide sites for attaching catalytically active species in an unsolvated environment. A host of solid-state designers are involved in the tailored synthesis of porous frameworks (2, 3).

By comparison, research into the design and synthesis of more conventional close-packed solids is not very fashionable. But this may change with the report by Atwood et al. on page 1000 of this issue. The authors show that a very common organic compound, a calixarene, forms an entirely nonporous solid-state structure yet allows rapid bulk diffusion of small molecules without losing its crystallinity (4).

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Calixarenes are well-studied molecules, and none more so than p-tert-butylcalix[4]arene (see the figure) (5, 6). The molecule adopts a bowl shape in both solid and solution phases, reminiscent of a Greek vase called a calyx crater (hence the name). The interior of the bowl can include small-molecule guest species such as toluene. A bewildering variety of calixarene host-guest compounds have been prepared (5, 6).

Atwood et al. have now crystallized the calixarene without anything inside the molecular cavity, simply by subliming the compound. The pure calixarene is difficult to obtain because of its propensity to include guest species, but is nothing spe-

cial in itself. The two known x-ray crystal structures (4, 7) of the guest-free calixarene show a close-packed solid much like the vast majority of compounds reported in the Cambridge Structural Database, albeit with relatively low densities (8).

The interesting step taken by Atwood et al. was to dip the ordered single crystal used in their x-ray study into liquid vinyl bromide. The solid calixarene is insoluble in vinyl bromide, but when the calixarene is cocrystallized from a solution in a different solvent it typically forms 1:1 host-guest complexes with a variety of guest molecules. Atwood et al. observed that this same kind of host-guest compound formed in a single crystal–single crystal phase transition over a period of about 15 min when the solid, guest-free calixarene was immersed without dissolution in the liquid vinyl bromide.
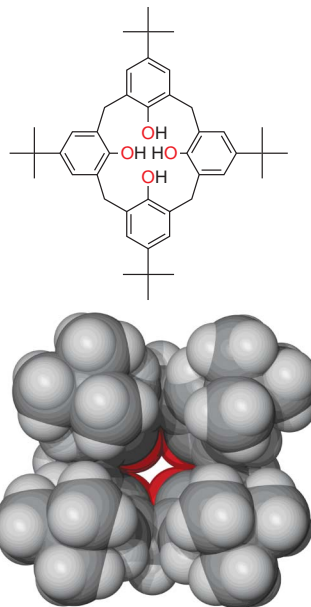
Well-studied yet full of surprises. (**Top**) p-tert-Butylcalix[4]arene. (**Bottom**) Space-filling plot of the calixarene's discrete molecular cavity.