polycrystals, are obtained when a Voronoi construction is used. Thus, the first important task in a simulation is to produce nanostructures that resemble closely what is experimentally synthesized.

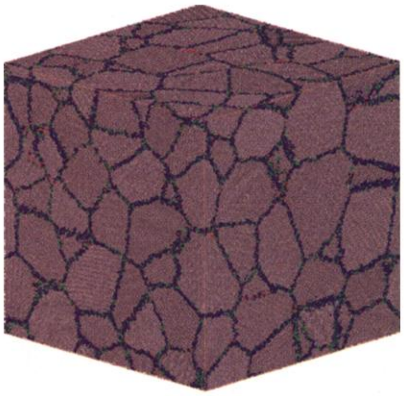
Most computer simulations have been performed on face-centered cubic metals. Large-scale molecular dynamics simulations have provided evidence for a transition, with increasing grain size, from intergranular plastic deformation based on grain boundary accommodation, to a mixture of intergranular and intragranular processes where the grain boundary acts as a source of imperfect or partial dislocations (*10–12*).

At the smallest grain sizes, room temperature simulations on samples with randomly distributed grains and grain orientations identified grain boundary sliding as the accommodation mechanism. The sliding is triggered by uncorrelated shuffling and to some extent by stress-assisted diffusion (*13*). On the other hand, simulations at higher temperatures on samples with symmetric grains and only high-energy grain boundaries, suggest that sliding is governed by enhanced grain boundary diffusion ("Coble creep") (*14*). The authors extrapolate Coble creep to room temperatures, on the basis of the presence of highly disordered grain boundaries. There is, however, no real justification for such an extrapolation, because it cannot be assumed that the rate-limiting process near the melting temperature also dominates at room temperature.

For larger grains (but still in the nanometer scale), grain boundary accommodation remains dominant, but grain boundaries start to also emit partial dislocations. As grain sizes increase, several partial or imperfect dislocations nucleate in different regions of the grain boundary, in contrast to the emission of full or perfect dislocations known from coarse grained metals (*15*).

Recently, full dislocations have been observed in simulations of columnar microstructures with grain sizes of 30 nm; plasticity was fully determined by dislocation activity (*16*). These samples are essentially two-dimensional, however, with only two slip planes for dislocations allowed. The energetics of a two-dimensional, infinitely extended dislocation structure are different from those of a full dislocation where the core line is pinned at both ends to a general grain boundary, and therefore the results cannot be compared.

Atomistic simulations of deformation are performed under high stresses and during very short deformation times (around 150 ps). It is often claimed that a steady-state strain rate is reached, justifying the calculation of activation energies. But this "steady state" is time-dependent. A reduction in strain rate by a factor of 10 has been observed when the simulation time was increased from 150 ps to 1 ns, a time still much shorter than in experiments. The rate-limiting processes addressed in these calculations are thus very dependent on the initial grain boundary structure and the loading conditions. During longer deformation times, many other processes take place in the grain boundary that change its structure during deformation. At room temperature, grain boundary structural relaxations toward lower energy structures have been observed, whereas at high temperatures, enhanced melting is to be expected.



Grain boundaries at the nanoscale. Computer-simulated sample of nanocrystalline Ni with a mean grain diameter of 10 nm. Each side of the box is 37 nm long, and the sample contains 4.6 million atoms. Gray atoms sit in perfect crystalline positions; colored atoms are grain boundary atoms.

Despite their limitations, the insight provided by simulations at the atomic scale is invaluable for guiding and understanding experimental results and for developing new theories. The future lies in a better understanding of the relation between grain boundary structures and their behavior under stress. Detailed knowledge of the relation between grain boundary structure and its mechanical behavior will allow the design of sophisticated microstructures and will lead to synthesis methods that produce improved grain boundary structures.

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PERSPECTIVES: PALEOCLIMATE

Trans-Atlantic Climate Connections

Paul A. Baker

Modern climate studies are limited by the short duration of instrumental records, particularly in the tropics. Modes of climate variability with periods greater than a few decades are only partially known and not well understood (*1*). If we are to understand tropical climate variability at longer time scales, we have to rely on proxy records such as those contained in lake sediments, reef corals, or high-altitude ice cores.

Several recent articles have sharpened the focus on the past and present climate of the tropics. On page 113 of this issue, Johnson *et al.* (*2*) describe a new sedimentary record spanning the past 25,000 years from Lake Malawi, one of the great lakes of tropical East Africa. Their discussion centers on finely-resolved biogenic silica in the record, a possible indicator of past precipitation. But equally impressive is their use of Nb/Ti as a fingerprint for volcanic ash, and benthic diatoms for reconstruction of past lake levels.

Disregarding as possible artifacts those silica peaks that coincide with the two Holocene ash events, two distinctive long-term climatic phases stand out. Low silica accumulation coincides with low lake level between 25,000 and 16,000 years before present (yr B.P.) and, again, between 13,000 and 11,000 yr B.P. After 11,000 years B.P., lake level and silica both increased to values maintained to the present.

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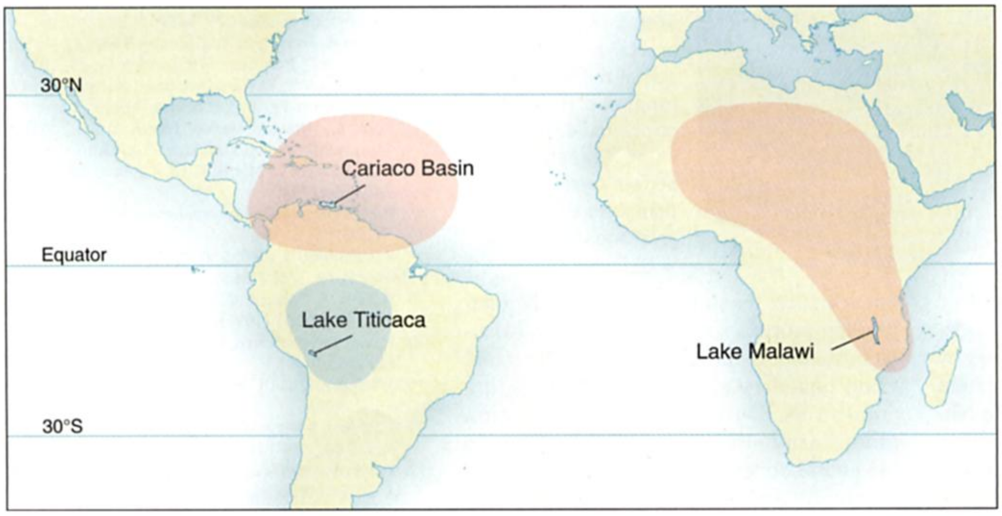
Important questions arise from these data and the few other long paleoclimatic records that exist for tropical Africa and America. To what extent does solar radiation force tropical precipitation amounts, compared to atmospheric CO_2 concentrations or other factors?

On time scales on the order of 10,000 years, radiation received at the top of the atmosphere (insolation) in the tropics is controlled primarily by the roughly 20,000-year periodic precession of the equinoxes. About 20,000 years ago, at the global Last Glacial Maximum (LGM), perihelion occurred when the Sun was directly over the southern subtropics in the austral summer wet season (as today), and summer insolation was 8% greater in the southern subtropics than 10,000 years later. At the LGM, southern tropical precipitation should have been enhanced and northern tropical precipitation should have decreased.

In tropical America, this expectation was fully realized (see the figure), with wet conditions dominant at the LGM in much of the southern tropics (*3*) and dry conditions dominant in the northern tropics (*4*). In the early Holocene, some 10,000 years later, southern tropical America was drier, and the northern tropics were wetter (*5*). Present-day precipitation in America has again reached a long-term high in the southern tropics and a low in the northern tropics.

In Africa, however, only the northern tropics appear to have behaved as expected on these long time scales. Northern tropical Africa was cold and dry at the LGM (*6*), substantially wetter during the so-called "early Holocene climatic optimum" (*7*), and, once again, more arid today. No sites with enhanced precipitation are known in southern tropical Africa at the LGM, and Johnson *et al.* (*2*) now rule out Lake Malawi (at 10° to 14°S) as such a candidate site. Instead, the climate of Lake Malawi was dry at the LGM.



Inferred distribution of tropical precipitation (*2–7, 10–13*) at the LGM (ca. 20,000 yr B.P.). Red signifies relatively dry conditions, blue relatively wet conditions. This pattern is also found for the Younger Dryas and perhaps the Little Ice Age; the same pattern, but with opposite signs, is inferred for the early Holocene (6000 to 10,000 yr B.P.).

It appears that glacial boundary conditions (low atmospheric CO_2 and CH_4 concentrations, low sea level, high-latitude glaciers, low sea surface temperature) prevailed over orbital control of insolation in southern tropical Africa (*6*), but not in southern tropical South America. It is even more puzzling (because glacial boundary conditions had already been replaced by near-preindustrial values) that southern tropical Africa was wet in the early Holocene.

On time scales of 100 to 1000 years, "abrupt" paleoclimatic events, recorded in sediments and ice cores mostly in the north Atlantic region, are also observed in the terrestrial tropics. Two of the best documented examples of such events in the past 25,000 years are the Younger Dryas (about 12,600 to 11,500 yr B.P.) and the Little Ice Age (about AD 1300 to 1850). Solar variability and volcanism appear to have forced the Little Ice Age (*8*), whereas the Younger Dryas seems to have resulted from changes in oceanic thermohaline circulation due to sudden inputs of glacial melt water to the North Atlantic (*9, 10*). Both manifested themselves at high northern latitudes as cold periods.

A marine sedimentary record from the Cariaco Basin clearly indicates that northern South America was dry during both the Younger Dryas and the Little Ice Age (*11*), whereas much of the southern tropics of South America was wet during both periods (*3, 12*). Perhaps relative warming of the south Atlantic Ocean brought about a southward migration of the atmospheric intertropical convergence zone in the Atlantic.

By contrast with South America, the Younger Dryas coincided with a dry phase in both northern and southern tropical Africa (*6*). If the Atlantic intertropical convergence zone migrated southward, it did so more in the eastern Atlantic than in the western Atlantic, becoming even more asymmetric than today. The signal of the Little Ice Age in tropical Africa was more complex or the existing records less definitive. But a remarkable covariation between biogenic silica in Lake Malawi sediments (*13*) and continental runoff recorded in Cariaco Basin sediments (*11*) supports the notion that the climates of tropical Africa and northern South America responded coherently to a nearly global-scale forcing.

The singular hydrologic response of tropical Africa (dry) and the mixed response of tropical South America (wet south, dry north) during northern high-latitude cold events such as the LGM and Younger Dryas, implies that the methane flux into the atmosphere is largely controlled by tropical Africa. This helps to explain a previously observed correlation between past African lake levels and the global methane record (*14*).

The report of Johnson *et al.* (*2*) provides an important piece in the puzzle of tropical climate patterns. It is particularly timely in light of a major new research initiative to undertake deep scientific drilling in Lake Malawi. Drilling is scheduled to begin in January 2003. Similar scientific drilling of Lake Titicaca in the high-altitude tropics of South America was completed in June 2001 (*15*). The goal of both projects is to extend paleoclimatic records of the tropics to perhaps the past million years in order to broaden the context for understanding modern climate variability.

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