

models are already helping experimenters to fill in the missing structural data from their x-ray crystallography and cryoelectron microscopy experiments and to tackle ever more challenging structure problems.

New drugs

One of the most important uses of protein structures is in drug development. To stop a protein from performing some harmful action in the body, pharmaceutical scientists study the protein's structure, identify a nook or cranny that may correspond to the protein's active site, and design a molecule to plug it up like a cork in a wine bottle.

"But there's really no such thing as 'the' structure," says Carnevale, because proteins flex and contort. Focusing on fitting a molecule to one static structure ignores all the other conformations a protein can adopt or the transitions between them, any one of which might offer a more effective way to disrupt the protein's function.

In some cases, the dynamic approach to drug development might be the only viable one. In neurodegenerative condi-

tions like Alzheimer's and Parkinson's diseases, amino-acid chains get tangled up and fold into the wrong structure, called an amyloid fibril. The fibril structure is known (see PHYSICS TODAY, June 2013, page 16), but the structure alone doesn't say much about how the fibril forms—or how to stop it from forming.

It would take a far more sophisticated model than the ones available today to predict a protein's entire conformational ensemble and range of motion. But as Carnevale points out, "Surely the sequence must encode that information, because nature knows what it is."

Another ambitious goal that's on Baek and colleagues' minds is to free their model from the need to consider evolutionary relationships at all and predict the folded structure based only on the amino-acid sequence. Evolution has produced a wondrous array of proteins and functions, but it hasn't come close to exploring every possible protein. The Baker lab's specialty is in designing proteins from scratch to do things that natural ones can't. (See PHYSICS TODAY, June 2020, page 17.) But those bespoke proteins don't come with millions of years of

evolutionary relatives to analyze.

Says Dill, "The whole field is headed toward bigger, better, faster": bigger proteins, more complex actions, and more detailed information than has ever been possible before. Lately, modelers and experimenters alike have been working on understanding the spike protein of SARS-CoV-2—the virus that causes COVID-19—whose binding to a host cell involves a cascade of large conformational changes.⁵ As Dill explains, "It's a huge protein that's part of an even huger complex, the virus, with all kinds of moving parts like a big Rube Goldberg machine."

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A seismometer maps Mars's anatomy

NASA's *InSight* is the first mission to explore seismic waves in a planetary body since *Apollo 17* in 1972.

On 26 November 2018, the *InSight* lander—whose acronym stands for Interior Exploration Using Seismic Investigations, Geodesy and Heat Transport—touched down on Mars's Elysium Planitia. Within two months on that flat, volcanic plain, the lander's robotic arm removed a seismometer from the lander deck and placed it on the ground (figure 1), where it started listening for vibrational signals. Eight orbiters currently survey the gravitational fields, magnetism, and atmosphere of Mars, and six rovers have explored its surface chemistry and geology. *InSight*'s seismometer is the only current direct probe of the planet's interior.

To date, the instrument has picked up more than 1000 distinct seismic events. Of the several hundred marsquakes it's recorded, the vast majority were small—none exceeded a moment magnitude of 4. A low level of seismic activity was not un-

expected. Unlike Earth, whose sharply defined tectonic plates intersect at boundaries that wind around the planet like the seam of a baseball, Mars has a single, thick plate.

The Martian activity, however, is even lower than what some planetologists expected for the thousands of faults that populate the surface. Most may have formed from stresses on the planet as it shrinks while slowly cooling. Some could have arisen from internal dynamics—mantle convection and volcanism.

The outer part of Mars solidified from a magma ocean produced by accretion early in solar-system history. An iron-rich core formed as heavy, molten metal sank into the planet's center and lighter, silicate-rich material rose; part of that lighter material melted and refroze into a brittle crust. Orbital measurements of the planet's gravity, tidal response, and moment of inertia provided early hints of that differentiation.

An international collaboration of 65 seismologists and planetary scientists from 12 countries has now published three papers that describe the first direct observations of those distinct layers.^{1–3} The teams' quantitative measurements of the structure set the stage for understanding how the planet evolved into its current thermochemical state.

Single seismometer

InSight isn't the first spacecraft to bring a seismometer to Mars. The two *Viking* landers each carried one when they landed on Mars in 1976. But uncaging mishaps and the seismometers' onboard installation prevented either from definitively detecting anything but the wind.

Working out planetary structure is largely a matter of interpreting shear (*S*) and compressional (*P*) seismic waves, which travel through the planet at different speeds and refract and reflect from the boundaries of the planet's layers. Those speeds vary with stiffness (or shear and bulk moduli, in geological parlance), density, and temperature. The difference in the waves' arrival times at the seismometer provides the distance to

a marsquake but not its specific location.

To locate the quake's epicenter, seismologists normally resort to triangulation using at least three seismometers. The distance from the quake is represented as a circle around each seismometer, and the epicenter lies at the intersection of the three circles. Beginning with *Apollo 11* in 1969, the Apollo program established a four-station seismometer network on the Moon. But seismologists couldn't afford a network on more distant Mars.

What's more, although it's surrounded by a protective shield to filter out wind-induced vibration, *InSight's* seismometer is still vulnerable to pressure vortices, daily temperature swings, and dust storms. Fortunately, Mars is naturally quiet. "Because it lacks oceans," says the Jet Propulsion Laboratory's Mark Panning, "it's at least two orders of magnitude quieter than any place on Earth in the 0.1–1 Hz frequency band that seismologists typically use." *InSight* is also sensitive enough that it can register vibrational amplitudes as small as an atomic width.

From the crust . . .

Marsquakes don't resemble the strong stick-slip interactions that take place at Earth's convergent plates. Rather, they mimic the slip along faults far from those boundaries. Tectonic fissures known as Cerberus Fossae (figure 2), which are located 1600 km from *InSight*, may account for the largest of that seismic activity.

Amir Khan of ETH Zürich and colleagues found that most marsquakes

take place in the shallow crust.¹ But as on Earth, *P* waves can partially convert to *S* waves on being reflected or refracted from discontinuities. And those conversions make individual waves difficult to disentangle. A smaller number of quakes appear to originate below the crust. Of the marsquakes the team recorded, the collaboration analyzed the eight cleanest events. From that sample, they extracted *P*- and *S*-wave arrival times and polarizations, which revealed the waves' directions. Armed with that additional polarization data, the seismologists *can* determine epicenter locations.

The University of Cologne's Brigitte Knapmeyer-Endrun and colleagues found distinct layer boundaries in the crust below the *InSight* lander.² The first, as deep as 10 km below the surface, marks a change in rock lithology. Either the second or third, as deep as 25 km and 47 km, respectively, marks the bottom of the crust. The latter thickness is more consistent with previous estimates from orbital surveys.

Data from seismic-wave reflections indicate that Mars's crust is quite porous—"more like the Moon than Earth," says David Stevenson, a planetary scientist not affiliated with the collaboration. That may be a consequence of being heavily altered by the meteor bombardment it suffered during its first billion years. With the new measurements, Knapmeyer-Endrun and colleagues used the crustal thickness under the lander as a calibration for mapping the crust across the entire planet. Mars's lithosphere, the rigid

outer part of the planet, reaches 400–600 km below the surface. That's more than twice as deep as Earth's continental lithosphere. And it's perhaps an indication of the upward migration of radioactive elements into the crust, which would reduce the average geothermal temperature gradient at depth.

. . . to the core

Simon Stähler of ETH Zürich and colleagues detected faint waves reflecting off the deeper core–mantle boundary.³ From their analyses of those reflections, they derived a core radius of 1830 km, about 100 km greater than expected, based on Mars's moment of inertia and mean density. The large size means that the core's composition is less dense than expected. And that, in turn, implies that a greater concentration of light elements, such as sulfur, carbon, silicon, and hydrogen, are sequestered there.

The enrichment in light elements would have lowered the core's melting temperature, possibly to a point that sustains the entire core as a molten liquid. If that's the case—and the lack of shear waves passing through the core suggests that it is—the absence of a solid inner core is likely one of the reasons Mars's dynamo turned off billions of years ago. Earth's dynamo is driven by latent heat from crystallization of the inner core, an energy source that is not available on Mars. But that's speculation. No one has yet measured how much heat flows from Mars's core.

With no dynamo to sustain it, Mars

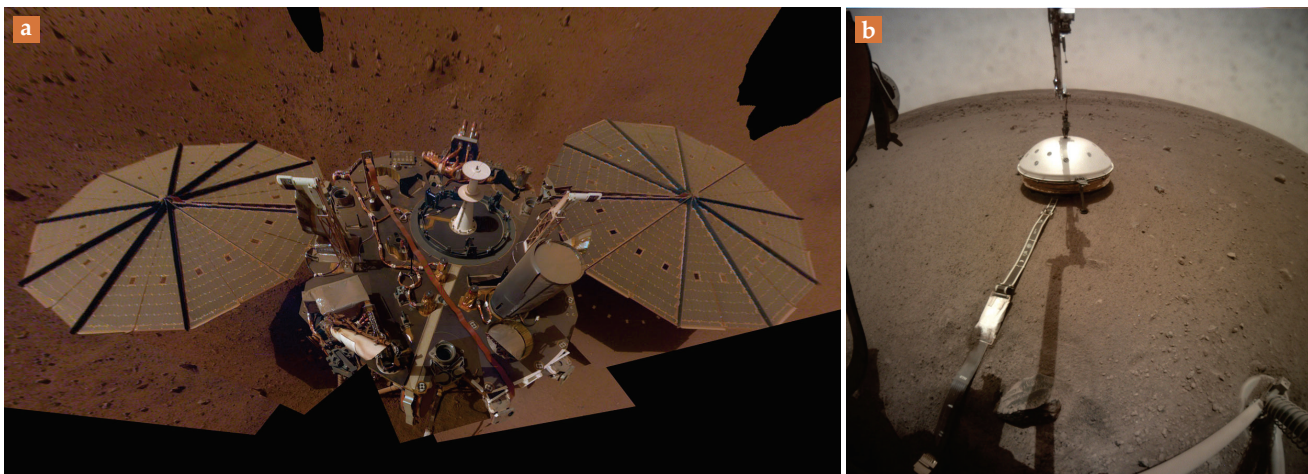


FIGURE 1. THE *INSIGHT* LANDER (a) took this selfie with a robotic arm in 2019 after unfolding its two solar panels (each one 4 m²) and placing its seismometer on the Martian surface. **(b)** Attached to the lander by an electrical cord, the seismometer is protected in a vacuum under a wind shield. (Courtesy of NASA/JPL-Caltech.)

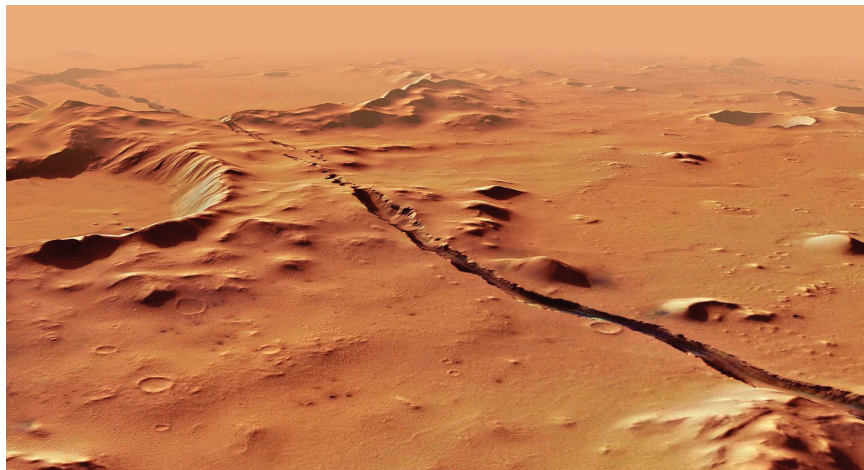


FIGURE 2. CERBERUS FOSSAE are a series of fissures on Mars formed by faults that are the source of several marsquakes. *InSight's* seismometer sits about 1600 km west. This photograph, which shows just one fissure, was taken by the European Space Agency's *Mars Express* orbiter. (Courtesy of ESA/DLR/FU Berlin, CC BY-SA 3.0 IGO.)

has no global magnetic field today. But it did early on. In 1997 an orbiting spacecraft discovered localized magnetic fields that were frozen into the oldest crustal rock shortly after the planet formed 4.5 billion years ago. How or when the planet's dynamo turned off is unknown, but it must have done so when heat leaking from the core had diminished sufficiently. (See the article by David Dunlop, *PHYSICS TODAY*, June 2012, page 31.)

The enrichment also aligns with what is suspected about the planet's early evolution. Isotope evidence from Martian meteorites on Earth suggests that Mars formed early in the outer regions of the terrestrial planetary zone, where light volatile elements might have been more available and incorporated into the planet while it was still an embryo. Hafnium–tungsten isotope analysis suggests that Mars formed roughly 5 million years after the solar nebula did; Earth formed some 30 million–40 million years later. (See the article by Bernard Wood, *PHYSICS TODAY*, December 2011, page 40.)

The large core size also influences the convection of heat from the mantle. Being proportionally thinner as a result of the large core, Mars's mantle never reaches the high pressures required to produce a stable phase transition from ringwoodite—a high-pressure phase of olivine—to bridgmanite. Also known as magnesium perovskite, bridgmanite is the most abundant mineral in Earth. It is widespread in Earth's mantle deeper than about 660 km and circulates more slug-

gishly than the mantle above. On Mars, the absence of bridgmanite might have allowed the core to cool more efficiently.

Before the *Spirit* and *Opportunity* rovers finally died, dust devils occasionally boosted their power levels by scouring dirt from the rovers' solar panels (see the Quick Study by Ralph Lorenz, *PHYSICS TODAY*, July 2020, page 62). *InSight's* lander has not enjoyed the same treatment—few devils appear in its vicinity—and its solar panels are producing just 27% of their dust-free power capacity. Mars is now close to aphelion, its farthest point from the Sun. Power is being shared among the spacecraft's science instruments, robotic arm, radio, and various heaters that keep everything working despite subfreezing temperatures.

Nevertheless, NASA expects the lander to survive the lower levels of sunlight and has extended the mission through December 2022. "We're still waiting for bigger quakes," says Panning. He and others are hoping for magnitude 5 events—larger signals would mean better resolution of core reflections, which would firm up constraints on deep structure. There's certainly more to learn. *InSight* has yet to detect any meteor impacts, for instance, despite predictions that it should see at least one a year.

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