Experiments at Atom-Crushing Pressures

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Experimentalists are now generating terapascal pressures in the laboratory, conditions sufficient to alter the structure of atoms and the nature of interatomic bonding (*1*). These are the pressures of planets' interiors and origins: 7 TPa at Jupiter's center, 4 TPa in the middle of Saturn, 0.36 TPa for Earth's inner core; and planetary accumulation involves impacts generating pressures into the terapascal range (*2*). Understanding materials and their properties at such conditions thus provides key insights into how planetary bodies form, and then evolve over billions of years. On page xxx of this issue, Fratanduono, et al. (*3*) establish a new calibration for terapascal experiments, and their pressure-volume relations for gold (Au) and platinum (Pt) can now serve as reliable standards to over 1 TPa.

This is a notable contribution because the forces that stabilize the atom are of terapascal magnitude. For example, the quantum mechanical pressure that keeps the negatively charged electron from being pulled into the positively charged nucleus of the Bohr atom is $\hbar^2/(4\pi m_e a_0^5)$ = 2.3 TPa, with $\hbar$, m_e and a_0 = 53 pm being Planck's constant/2π, the mass of the electron and the Bohr radius. Current experiments can therefore overwhelm ambient-condition quantum forces, and profoundly change the properties of materials.

For comparison, the pressure–volume work associated with compression to million-atmosphere (0.1 TPa) pressures amounts to electron-volt changes in a material's energy: enough to affect the outer bonding electrons, hence the chemical properties of atoms (*4*). The trends of the Periodic Table become distorted under these conditions, with xenon, oxygen and fluid hydrogen all transforming to metals, and the "simple metal" sodium becoming a transparent, ionic salt (electride) by 0.2 TPa (*5, 6*). The more extreme conditions at the atomic unit of pressure, E_H/a_0^3 = 29 TPa, alter the internal energy of materials by kilo-electron volts (*7*). This is the gateway to "kilovolt chemistry" in which core electrons – the deeper electron orbitals of the atom – engage in chemical bonding (*2, 8*).

Already, first-principles quantum mechanical calculations predict unusual properties at multi-terapascal pressures, for instance with the stabilization of relatively open crystal-structure geometries for elemental iron as well as for a variety of compounds, despite the atoms being under high compression (*8-10*). Hydrogen is expected to be a metallic quantum-crystal at these conditions, with atomic separations approaching the de Broglie wavelength (i.e., atoms becoming quantum indistinct), and the liquid state may exhibit exotic combinations of superconductivity and superfluidity (*11*).

Motivated by these predictions, experimentalists have stretched their capabilities to achieve record high pressures under controlled laboratory conditions. Diamond-anvil cells are now approaching 1 TPa by compressing samples between cleverly sculpted diamond tips, holding the ~ 1 μm^3 (1 femtoliter) sample for – as far as we know – arbitrarily long periods of time (*12*). Room-temperature superconductivity was recently reported in a carbonaceous sulfur hydride compressed inside a diamond cell to 0.3 TPa (*13*); the impact on technology could be huge, if it leads to the synthesis of ambient-condition superconductors. In contrast, pulsed power- and laser-driven dynamic-compression can characterize much larger (cubic millimeter sized) samples to far higher pressures, but only for tens to hundreds of nanoseconds. For example, laser-driven ramp loading – in principle a nearly isentropic compression – has taken carbon to 5 TPa, into the Thomas-Fermi-Dirac statistical atom regime, and spherically converging shocks have produced equation-of-state data to nearly 50 TPa: conditions relevant to understanding white dwarfs (*14, 15*).

The diversity of techniques is notable, with a variety of static versus dynamic means of generating high pressures, and experimental diagnostics ranging from velocity interferometry to x-ray diffraction and spectroscopy. Calibration has thus become essential for comparing the different laboratory measurements, all the more so as the samples are probed over different temperatures and timescales by the different high-pressure methods. Fratanduono, et al.'s pressure–volume measurements using both pulsed-power and laser-driven compression showed that the two technologies – which can differ by an order of magnitude or more in sample dimensions and compression time – are in good agreement with each other (*3*). They also find general accord with the diamond-anvil reports, but are able to provide improvements for the necessarily extrapolated calibrations of past experiments.

It is comforting yet almost amazing that measurements made over timescales spanning 12 orders of magnitude, from 10^{-8} s for laser-driven compression to 10^{4} s or more for static high-pressure experiments, are in such good agreement with each other. The power of calibration is in allowing completely independent experiments to be compared and even combined, not only validating but substantially enhancing the results because each method has its advantages and drawbacks. Short duration invites non-equilibrium effects in the dynamic measurements, whereas small samples and large stress gradients challenge reproducibility and quantification in the static experiments.

One of the key reasons that robust calibration is essential is that these experiments provide tests of first-principles quantum mechanical calculations of material properties. To be clear, theory and experiment are closely symbiotic, with the laboratory work being guided by quantum calculations, which also help in the interpretation and application of the experimental results. At the same time, experiments provide important validation for theory, and discrepancies between theory and experiment help guide improvements in both. Working at extreme conditions, the community is moving toward more reliable predictions of material properties and phase stability at ambient conditions, thereby advancing technology as well as fundamental understanding. The work also helps us better understand planets, the platforms on which life can establish itself and evolve.

1) One terapascal corresponds to 10 million atmospheres pressure.
2) R. Jeanloz, et al., *Proc. National Acad. Sci.*, **104**, 9172-9177 (2007).
3) D. E. Fratanduono, et al., *Science*
4) 1 eV = 96.5 kJ/mol
5) Y. Ma, et al., *Nature*, **458**, 182-185 (2009).
6) The electron charge density becomes concentrated between the sodium ion cores at high pressure, such that the element effectively transforms into the “salt” Na^+e^-, with Na^+ cations bound to e^- “anions” of increased charge density but without a nucleus.
7) Hartree’s atomic unit of energy, $E_H = \hbar^2/(m_e a_0^2)$ = 27 eV, is the kinetic + potential energy of the Bohr atom, and the unit of pressure is simply the energy density E_H/a_0^3 derived on dimensional grounds.
8) M. Miao, Y. Sun, E. Zurek and H. Lin, *Nature Revs. Chem.*, **4**, 508-527 (2020).
9) C. J. Pickard and R. J. Needs, *J. Phys.: Condens. Matter*, **31**, 452205 (2009).
10) L. Stixrude, *Phys. Rev. Lett.*, **108**, 055505 (2012).
11) J. E. McMahon, M. A. Morales, C. Pierloni and D. M. Ceperley, *Rev. Modern Phys.*, **84**, 1607-1653 (2012).
12) N. Dubrovinskaia, et al., *Sci. Adv.*, **2**: e1600341 (2016).
13) E. Snider, et al., *Nature*, **586**, 373-377 (2020).
14) R. F. Smith, et al., *Nature*, **511**, 330-333 (2014).
15) A. L. Kritcher, et al., *Nature*, **584**, 51-54 (2020).
16) Acknowledgements. I have benefitted from discussions with G. W. Collins, D. E. Fratanduono, N. Y. Yao and E. Zurek. Work supported by the NNSA Center for Matter under Extreme Conditions and the NSF Physics Frontier Center for Matter at Atomic Pressure.

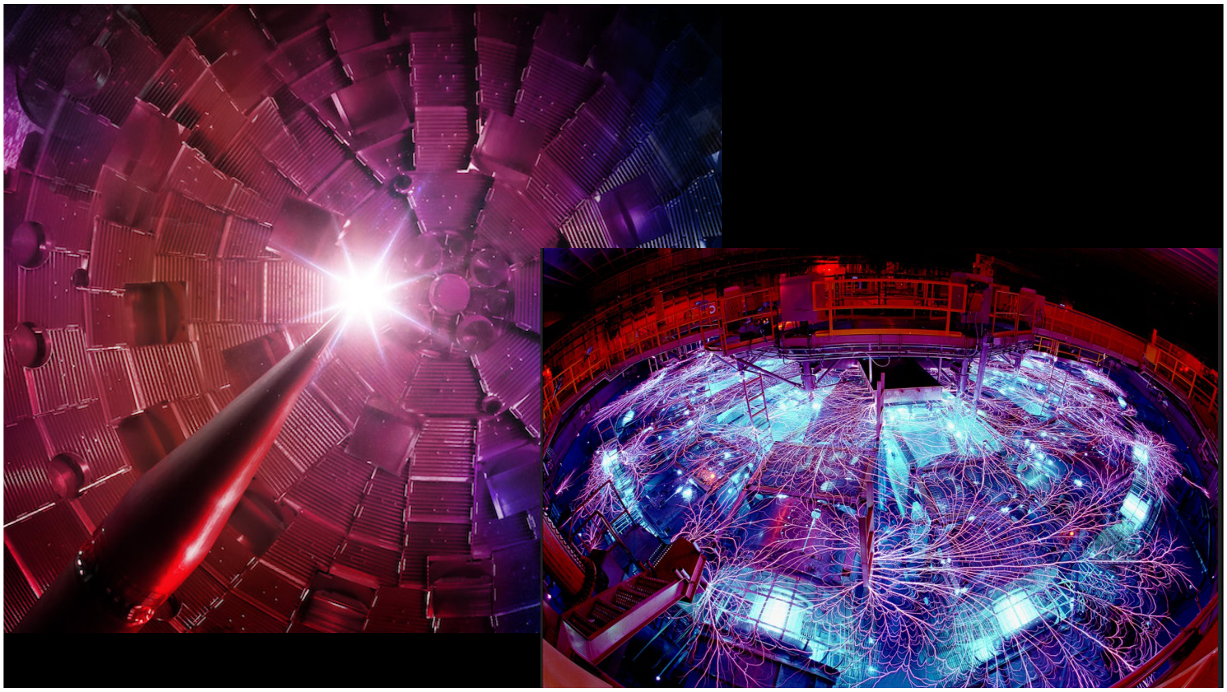

Fig. 1. Measurements at the National Ignition Facility (NIF, *left*) and the Z pulsed-power facility (*right*) provided the means of calibrating high-pressure experiments to terapascal pressures. The spherical target chamber at NIF is 3 stories high (10 m), and the diameter of the Z machine is nearly 4 times larger (37 m).