

of mesoscopic materials by developing multiscale simulation techniques, particularly in electronics, because, for example, conventional approaches break down for nanoscale devices, and first-principles-based approaches are computationally costly.

Considering the importance and difficulties faced in this research field, the government should invest more in the necessary resources required for success, including platforms for high-throughput

computational searches, rapid experimental synthesis and characterization facilities, and databases of material structures and properties. These features are all part of the MGI in the United States, and presents researchers with opportunities to take computational research to the next level. Although infrastructure is gradually falling into place, more will need to be done to ensure that computational materials science in China can be successful in obtaining improved materials. □

Hai-Qing Lin is at the Beijing Computational Science Research Center, Haidan, Beijing 100193, China.
e-mail: haiqing0@csrc.ac.cn

References

1. Xie, X. *Acta Phys. Sin.* **14**, 164–190 (1958).
2. Li, J., Duan, C. G., Gu, Z. Q. & Wang, D. S. *Phys. Rev. B* **57**, 6925 (1998).
3. Chen, C. T. *et al. Adv. Mater.* **11**, 1071–1078 (1999).
4. Lin, Z. S. *et al. J. Phys. D.* **47**, 253001 (2014).
5. Yang, J.-H. *et al. Nano Lett.* **16**, 1110–1117 (2016).
6. Wang, Z. *et al. J. Am. Chem. Soc.* **137**, 9146–9152 (2015).
7. Zhang, S., Zhao, S., Kang, W., Zhang, P. & He, X.-T. *Phys. Rev. B* **93**, 115114 (2016).

High pressure presses ahead

Ho-kwang Mao discusses the history of high-pressure research in China, and recent developments to ensure further success.

Pressure is a fundamental thermodynamic variable that can dramatically alter the atomic and electronic structure of materials, resulting in concomitant changes to their properties. Generation of static pressure greater than 100 GPa in diamond anvil cells, and a growing number of associated in-laboratory and large facility-based probes worldwide, enables a broad pressure-induced phase space to be explored. These developments have permitted new physical understanding of a range of phenomena, not limited to what is going on in the Earth's core and celestial bodies, and pressure-induced

changes in elastic, electronic, magnetic, structural and chemical properties of materials. However, vast unexplored territory remains, and high-pressure research has substantial potential for unearthing new behaviours of materials. It therefore represents an attractive opportunity for China to demonstrate its capabilities in an international scientific field.

China has traditionally been very active in high-pressure research. This has been driven in part by China lacking natural diamond resources, yet some industries in China, including hard-rock drilling and

high-precision machining, rely on diamonds for superhard tools, synthesized by high-pressure routes. Moreover, knowledge of the dynamic compression of materials is relevant to Chinese defence science. As such, high-pressure research was relatively well protected throughout the tumultuous years of the Cultural Revolution (1966–1976), when other academic research fields essentially came to a halt. China has since grown to be the predominant manufacturer of the world's synthetic diamond abrasives.

To sustain the rapid economic growth experienced in China over the last few decades, international competitiveness in basic science has become increasingly crucial, and funding from the Chinese government towards this goal has been substantial. Materials science holds significant potential in this regard, and high-pressure research contributes to materials applications in three aspects. First, useful high-pressure phases, such as superhard diamonds and cubic boron nitride, can be synthesized directly under compression and preserved for ambient applications. Second, knowledge gained in high-pressure research may lead to alternative routes for the design and synthesis of high-pressure phases with useful properties. For instance, large single-crystal diamonds with ultrahigh purity can now be synthesized under low pressures using methods based on chemical vapour deposition¹. Third, the ubiquitous impact of pressure on physical behaviour provides an indispensable shortcut for advancing basic understanding. Thus, high-pressure research has stood out as one of the key directions of study that the Chinese government is supporting.



Figure 1 | An artist's impression of the Center for High Pressure Science and Technology Advanced Research headquarters that is currently under construction in Beijing (due to be completed in October 2017).

Resultantly, Chinese research institutions and universities are making seminal contributions to high-pressure science and technology. For example, the National Key Laboratory of Shock Wave and Detonation Physics, China Academy of Engineering Physics studied the density and sound velocity of Fe–O–S alloys under extreme pressure–temperature conditions, leading to the suggestion that the Earth's liquid outer core is depleted of oxygen². Meanwhile, researchers at the Institute of Physics, Chinese Academy of Sciences investigated the effect of pressure on the superconductivity of newly discovered doped iron chalcogenide superconductors^{3,4}, reporting a high re-emerging critical temperature of 48 K, the largest yet observed in this material class.

Jilin University has established itself as the leading high-pressure research centre in China since the 1960s. They recently made the astonishing discoveries that pressure could transform elemental sodium from a free-electron gas metal to a transparent insulator⁵, and that pressure could crush C₆₀ cages to form a new type of material with long-range ordering of short-range, disordered carbon clusters⁶. Meanwhile, researchers at Yanshan University made breakthroughs in the high-pressure synthesis of ultrahard nanotwinned cubic boron nitride⁷ and nanotwinned diamond⁸, and researchers at Zhejiang University reported pressure-induced devitrification of Ce₃Al — a seemingly disordered metallic glass — to a single crystal⁹.

To build on and accelerate advances in China, the Center for High Pressure Science and Technology Advanced Research (HPSTAR) was established as a top team of the Chinese Thousand Talents Program in 2013. It is modelled after the Carnegie Institution of Washington, with the same mission statement of supporting exceptional individuals to encourage investigation, research and discovery in the broadest and most liberal manner (www.carnegiescience.edu/about/mission).

HPSTAR is strategically set up with its central laboratory in Beijing (Fig. 1) next to the Beijing Computational Science Research Center, with the Shanghai laboratory next to the Shanghai Synchrotron Radiation Facility, and a further branch on the Jilin University campus. In addition, there is a virtual laboratory consisting of a team of scientific staff employed by HPSTAR, who collaborate with synchrotron facilities around the world to pioneer cutting-edge high-pressure X-ray technology. They devote significant time and equipment on-site, forming a large network in the United States and in Asia, providing HPSTAR scientists with ample access to major synchrotron facilities.

HPSTAR adopts common practices, which enabled some of the aforementioned breakthroughs, namely theoretical–experimental interaction, interdisciplinary approaches, international collaboration and utilization of central facilities crucial for high-pressure research. Including those mentioned previously, these practices have already resulted in a number of discoveries: observation of dislocation flow in 3-nm nickel crystals, in contrast to previous theoretical predictions that dislocations would be inactive for crystals below 10–30 nm¹⁰; measurement of the pressure-induced change of dihedral angles of molten iron in a crystalline silicate matrix via a 30-nm X-ray tomography probe, simulating the formation mechanism of the early Earth's core¹¹; development of a new X-ray microprobe integrated with multigrain crystallography, used for the discovery of a key mineral at the Earth's core–mantle boundary¹²; and discovery of a new FeO₂ phase which may provide an explanation as to the origin of our oxygen atmosphere¹³.

HPSTAR's open, flexible and liberal research system is alien to the rigid Chinese system, and has thus faced numerous hurdles, including visa and work permit obstacles for foreign staff, and residency

requirements for Chinese employees on the municipal level. Nevertheless, it has thus far proven to be an effective system for significant breakthroughs, and has gained strong support from the Chinese central government, and more widely from the scientific community. Of particular note is that HPSTAR has been successful in attracting international researchers with non-Chinese origins, something that has traditionally been difficult to achieve in China, yet seen as important in diversifying the researcher pool in the country.

China has established itself as a strong figure in high-pressure research, providing a striking example of how China-based research groups can influence and lead global scientific research efforts. With substantial investment in many of the key facilities needed for high pressure research — including the China Spallation Neutron Source that is currently under construction — and an ongoing drive to attract the best researchers, China is in an excellent position to play a key role in advancing high-pressure science and technology, providing these enabling trends continue. □

Ho-kwang Mao is at the Center for High Pressure Science and Technology Advanced Research, Shanghai 201203, China and at the Carnegie Institution of Washington, Washington DC, USA. e-mail: maohk@hpstar.ac.cn

References

- Meng, Y.-f. *et al.* *Phys. Status Solidi A* **209**, 101–104 (2012).
- Huang, H. *et al.* *Nature* **479**, 513–516 (2011).
- Sun, L. *et al.* *Nature* **483**, 67–69 (2012).
- Guo, J. *et al.* *Phys. Rev. Lett.* **108**, 197001 (2012).
- Ma, Y. *et al.* *Nature* **458**, 182–185 (2009).
- Wang, L. *et al.* *Science* **337**, 825–828 (2012).
- Tian, Y. *et al.* *Nature* **493**, 385–388 (2013).
- Huang, Q. *et al.* *Nature* **510**, 250–253 (2014).
- Zeng, Q. *et al.* *Science* **332**, 1404–1406 (2011).
- Chen, B. *et al.* *Science* **338**, 1448–1451 (2012).
- Shi, C. Y. *et al.* *Nature Geosci.* **6**, 971–975 (2013).
- Zhang, L. *et al.* *Science* **344**, 877–882 (2014).
- Hu, Q. *et al.* *Nature* <http://dx.doi.org/10.1038/nature18018> (2016).

Corrected after print: 1 July 2016

Microscopy sparks development

Electron microscopy has seen a massive boom in China. Ze Zhang and Xiaodong Han discuss what this could mean for materials research and development.

China's rapid development over the last few decades has led to the production of huge quantities of materials, for both domestic and international markets. For example, China accounts for more

than half of the worldwide production of materials such as ferrous and non-ferrous metals, concrete and synthetic fibres^{1,2}. However, due to a lack of exact microstructural control, or a complete

understanding of the underpinning science, China has been unable to produce many high-end materials. Thus — at considerable cost — China must import millions of tons of high-quality specialty steels each year³

Correction

In the version of the Feature 'High pressure presses ahead' originally published (*Nature Mater.* **15**, 694-695; 2016), in the sentence beginning 'To build on and accelerate advances in China...', the year should have been 2013 and not 2003. Corrected in the online versions 1 July 2016.