

## Superconductivity with Tc as high as 32K found in borides

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The superconducting phase diagram of MoB2 as a function of the pressure is summarized in the Figure. Utilizing Diamond Anvil Cell (DAC) (left), it can be seen that the superconducting state emerges around 20 GPa, and then the Tc increases further with applied pressure, and beyond the structure-transition pressure (Pc ~ 70 GPa) the growth of Tc slows down. The Tc of MoB2 rises to as high as ~32 K at a pressure of 109.7 GPa and still does not exhibit the trend of saturation. Further theoretical calculations suggest that the out-of-plane phonon mode of Mo atoms couples strongly with Mo d electrons near EF (right). These results reveal the study of superconducting mechanism in high-pressure  $\alpha$ -



MoB2 sheds light on exploring of new phonon-mediated high-Tc superconductors in transition metal borides. Credit: Science China Press

Superconductors with high transition temperature (high- $T_c$  SCs) are longsought targets in the condensed matter physics and materials communities because of significant scientific and application values. Since the discovery of superconductivity in mercury more than one hundred years ago, only a handful of systems show  $T_c$  higher than 30 K.

Scientists at the ShanghaiTech University and their collaborators at Renmin University of China discovered superconductivity up to 32 K in  $MoB_2$  under pressure, which is the highest  $T_c$  in transition-metal borides up to now. Their findings, published in the journal *National Science Review*, shed light on the exploration of high- $T_c$  superconductors in transition metal borides.

Molybdenum diboride (MoB<sub>2</sub>) is unique among the MB<sub>2</sub> family since it is the only material that has two structural forms,  $\alpha$ -MoB<sub>2</sub> phase (AlB<sub>2</sub>-type) and  $\beta$ -MoB<sub>2</sub> phase (CaSi<sub>2</sub>-type).

Synchrotron X-ray diffraction (XRD) measurements indicate that  $\beta$ -MoB<sub>2</sub> transforms to  $\alpha$ -MoB<sub>2</sub> at around 65 GPa, which possesses the same <u>crystal structure</u> as MgB<sub>2</sub>.

"A question arises naturally: is it possible to achieve superconductivity in MoB<sub>2</sub> under <u>high pressure</u>?" said Dr. Yanpeng Qi, an assistant professor of School of Physical Science and Technology at ShanghaiTech University and one of the corresponding authors.

"So, we carried out the in-situ high pressure electrical transport measurements. Superconductivity is observed at 21.7 GPa and  $T_c$ 



increases with pressure. Beyond the critical pressure ( $P_c = 70$  GPa) where the structural phase transition, the growth of  $T_c$  slows down and the maximum  $T_c$  of 32.4 K is attained at P = 109.7 GPa, which is the highest pressure we exert on the sample."

Further theoretical calculations suggest that although the compressed  $MoB_2$  has a similar structure and comparable  $T_c$  with MgB<sub>2</sub>, the superconducting mechanism of the former is completely different from that of the latter: the d-electrons and phonon modes of transition metal Mo atoms play utterly important roles in the emergence of superconductivity in contrast to the dominance of p-electrons and phonon modes of B atoms in the superconductivity of MgB<sub>2</sub>.

The results shown in this work highlight the roles of transitional metals in the superconductivity in borides, which has been underestimated in borides before. Their discovery of superconductivity of  $MoB_2$  with rather high  $T_c$  could also shed light on the exploration of high- $T_c$ superconductivity in systems with light elements considering the synergic effects of light elements with high frequency phonon modes and strongly correlated electrons in transition metals.

**More information:** Cuiying Pei et al, Pressure-induced Superconductivity at 32 K in MoB2, *National Science Review* (2023). DOI: 10.1093/nsr/nwad034

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