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Gleb Parakhonskiy (left) and Elena Bykova (right), doctoral students in the program „Experimental Geosciences“ of BayNAT, the Bayreuth Graduate School of Mathematics and Sciences.
In between their supervisors at the University of Bayreuth, Prof. Dr. Natalia Dubrovinskaia and Prof. Dr. Leonid Dubrovinsky.

New industry-relevant findings in boron research

A research team at the University of Bayreuth succeeded in positively identifying alpha-boron as thermodynamically stable phase of boron. Furthermore, the findings, which are published in the latest issue of “Scientific Reports”, provide a basis for the possible production of single crystals of alpha-boron with the help of high pressure technology on an industrial scale. This opens up new prospects for industrial applications, especially for the semiconductor industry and the generation of solar power.

Discovered in 1808, boron is one of the most enigmatic chemical elements. Because of its extremely high reactivity, it does not exist in pure form in nature. Pure boron crystals

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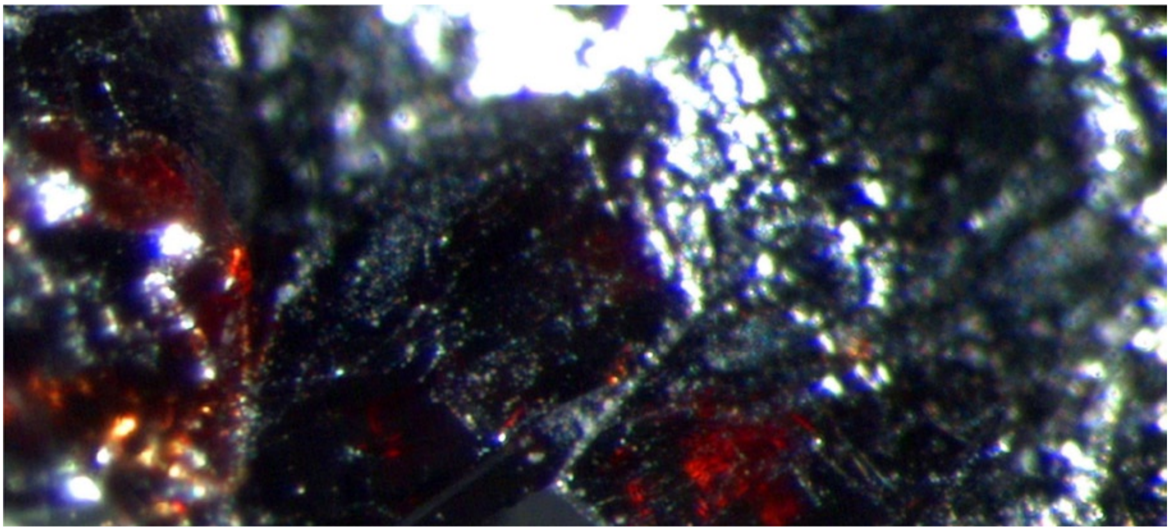

Alpha-boron crystals with a length of about 2 mm under an optical microscope.
A number of physical properties of alpha-boron are of particular interest for technical applications: it is a wide band gap semiconductor distinguished by its high hardness, heat resistance and comparatively low density.

can be produced artificially under high pressures and temperatures. Depending on the pressure and temperature conditions, this process results in synthesis of three different types of boron crystals which are called “phases” in research. They differ from each other in their structures, which are of varying complexity, and are called alpha-, beta- or gamma-boron.

Researchers have long disagreed on a question that is highly relevant both for basic research and technical applications: what is the most stable phase of boron? A team led by Prof. Dr. Natalia Dubrovinskaia, Heisenberg professor for Materials Physics and Technology at the University of Bayreuth, and Prof. Dr. Leonid Dubrovinsky at the Bavarian Geoinstitute (BGI) was able to clearly settle this dispute in favour of alpha-boron. What is more, their joint research efforts in Bayreuth and Potsdam (the GeoForschungsZentrum Potsdam is also involved in the boron project) found out that modern high pressure technologies could presumably be adapted to produce alpha-boron on an industrial scale. The researchers from Bayreuth and Potsdam report on their findings in the latest issue of “Scientific Reports”.

A series of various boron crystals was synthesized in the high-pressure labs of the BGI, a research centre at the University of Bayreuth, at temperatures of up to 2300 degrees Kelvin (ca. 2030 degrees Celsius) and pressures of up to 15 gigapascals. A favourite comparison demonstrates how extraordinary these artificially produced conditions are: if one could balance the Eiffel Tower on a fingertip, this would correspond to a pressure of 10 gigapascals. Alpha-boron crystals were synthesized at pressures between 4 and 11 gigapascals in combination with temperatures between 1400 and 1900 degrees Kelvin. The data gained from experiments led to the conclusion that alpha-boron – and not crystals of beta-boron, as many assumed – is the most stable phase of boron.

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At the same time the researchers succeeded in characterizing the alpha-boron crystals synthesized in the lab more precisely. A number of properties of particular interest for technical applications were either confirmed or for the first time reliably proven through highly precise measurements: alpha-boron is a wide band gap semiconductor distinguished by its high hardness, heat resistance and comparatively low density.

What is especially interesting for research and industrial applications is single crystals of boron. A single crystal solid is a material in which the crystal structure of the entire sample is continuous and unbroken to the edges of the sample, with no grain boundaries. The absence of the defects associated with grain boundaries can give the single crystals unique properties, particularly mechanical, optical and electrical. These properties, in addition to making them precious in some gems, are industrially used in technological applications, especially in optics and electronics. Until now, in-depth research on the application potential of alpha-boron had mainly been hampered by the fact that there was no reliable process to synthesize single crystals of alpha-boron. This impediment has now been eliminated. The paper published in “Scientific Reports” contains a phase diagram showing stability fields of boron phases with different properties and structures. Therefore, recommendations are now available for the targeted production of boron crystals, including single crystals of alpha-boron.

The research results produced at the University of Bayreuth open up the possibility of using boron crystals for innovative applications in various branches of technology. Alpha-boron, which can probably be produced on an industrial scale, is a highly attractive material especially for the semiconductor industry. In addition, it may be suitable for the construction of solar panels that convert sunlight into electrical energy with a high level of efficiency.

Publication:

Gleb Parakhonskiy, Natalia Dubrovinskaia, Elena Bykova,
Richard Wirth, Leonid Dubrovinsky,
Experimental pressure-temperature phase diagram of boron:
resolving the long-standing enigma,
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