Scientists about the Negative Thermal Expansion in Lithium Metaborate Crystals

Negative thermal expansion (NTE) is considered a rather unusual behaviour for solids. In most cases, substances expand when heated. Atoms of solids begin to oscillate with larger amplitude in the crystal lattice and occupy a larger volume. Many liquids and gases behave in the same way. Contrary to this logic, there are substances in the world that have a negative coefficient of thermal expansion: ordinary ice is considered a striking example of this behaviour. Chinese and Russian researchers have studied the NTE behaviour of layered materials to understand how to better manage 2D NTE materials or composites containing such materials.

> *"In this study, we observed two-dimensional (2D) NTE behaviour in a lithium metaborate ($LiBO_2$) crystal occurring inside graphite-like layers. We found out that this behaviour is due to an unusual decrease in the angles ∠O-Li-O and ∠B-O-B inside these layers, which in turn is caused by an increase in the lengths of the Li-O bonds with increasing temperature,"* said **Maxim Molokeev**, co-author of the article, assistant professor at the Basic Department of Solid State Physics and Nanotechnologies of the School of Engineering Physics and Radioelectronics, Siberian Federal University.

Lithium metaborate is a well-known inorganic compound — a salt of lithium and metaboric acid with the formula $LiBO_2$ — in the form of colourless crystals highly soluble in water and forming crystalline hydrates. The ease of synthesis, as well as the availability of starting materials, makes it possible to consider these crystals as interesting objects for studying two-dimensional NTE. The scientists were also interested in the prospects for the use of $LiBO_2$ in optics, because materials with negative thermal expansion have a very wide range of applications in technology, electronics, construction, medicine and, of course, photonics.

> *"Mixing $LiBO_2$ with a material that has normal thermal expansion can give various zero-expansion composite materials to stabilize the temperature swing effect. For example, dental fillings and tooth enamel expand at different rates when a person drinks hot tea. If fillings were made from a zero-expansion composite, this would solve the problem of pain that occurs as a reaction to a hot drink. As for optics, materials with well-controlled thermal expansion are also needed there. For example, the thermal conductivity of materials is of great importance for maintaining the thermal balance in laser optics applications, as well as in the design of optical lenses and substrates,"* **Maxim Molokeev** continued.

An interesting result of the work was the discovery of the fact that in a lithium metaborate crystal, the decisive role in the 2D-NTE behaviour is played by approximately the same stretching of Li-O both in the plane of the layer and outside of the plane. This made it possible to reconsider the prevailing opinion that the interlayer interaction should be much weaker than the intralayer one and significantly expanded the field of study of NTE materials.

Having studied the optical transmittance of the LiBO2 crystal, the scientists found that this material has high transparency in the range of 190-5790 nm at room temperature and has a wide spectral range (from ultraviolet to infrared radiation). Calculations show that a wide range of optical transmission will be maintained even with a change in temperature, which is very important for a material used in optics. Due to the advantage of 2D-NTE combined with excellent optical properties, LiBO2 will find wide application in ultra-precise optical devices operating at low temperatures.

Article

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