Substances trapped in nanobubbles exhibit unusual properties

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Skoltech scientists modeled the behavior of nanobubbles appearing in van der Waals heterostructures and the behavior of substances trapped inside the bubbles. In the future, the new model will help obtain equations of state for substances in nano-volumes, opening up new opportunities for the extraction of hydrocarbons from rock with large amounts of micro- and nanopores. The results of the study were published in the *Journal of Chemical Physics*.

The van der Waals nanostructures hold much promise for the study of tiniest samples with volumes from 1 cubic micron down to several cubic nanometers. These atomically thin layers of two-dimensional materials, such as graphene, hexagonal boron nitride (hBN) and dichalcogenides of transition metals, are held together by weak van der Waals interaction only. Inserting a sample between the layers separates the upper and bottom layers, making the upper layer lift to form a nanobubble. The resulting structure will then become available for transmission electron and atomic force microscopy, providing an insight into the structure of the substance inside the bubble.

The properties exhibited by substances inside the van der Waals nanobubbles are quite unusual. For example, water trapped inside a nanobubble displays a tenfold decrease in its dielectric constant and etches the diamond surface, something it would never do under normal conditions. Argon which typically exists in liquid form when in large quantities can become solid at the same pressure if trapped inside very small nanobubbles with a radius of less than 50 nanometers.

Scientists led by professor Iskander Akhatov of the Skoltech Center for Design, Manufacturing and Materials (CDMM) built a universal numerical model of a nanobubble that helps predict the bubble's shape under certain thermodynamic conditions and describe the molecular structure of the substance trapped inside.

"In a practical sense, the bubbles in the van der Waals structures are most often regarded as flaws that experimenters are eager to get rid of. However, from the standpoint of straintronics, the bubbles create strain, and its effect on the electronic structure can be used to create practical devices, such as transistors, logic elements and ROM," Petr Zhilyaev, a senior research scientist at Skoltech, said.

"In our recent study, we created a model which describes a specific shape that flat nanobubbles assume in the subnanometer dimension range only. We discovered that the vertical size of these nanostructures can only take discrete values divisible by the size of the molecules trapped. In addition, the model enables changing the size of nanobubbles by controlling the temperature of the system and the physicochemical parameters of the materials," said senior research scientist Timur Aslyamov.

More information: T. F. Aslyamov et al. Model of graphene nanobubble: Combining classical density functional and elasticity theories, *The Journal of Chemical Physics* (2020). DOI: 10.1063/1.5138687

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