'Quasicrystal' metal computer model could aid ultra-low-friction machine parts

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Duke University materials scientists have developed a computer model of how a "quasicrystal" metallic alloy interacts with a gas at various temperatures and pressures. Their advance could contribute to wider applications of quasicrystals for extremely low-friction machine parts, such as ball bearings and sliding parts.

Quasicrystals, like normal crystals, consist of atoms that combine to form structures -- triangles, rectangles, pentagons, etc. -- that repeat in a pattern. However, unlike normal periodic crystals, in quasicrystals the pattern does not repeat at regular intervals. So, while the atomic patterns of two crystalline materials rubbing together can line up and grind against one another, causing friction, quasicrystalline materials do not, and thus produce little friction.

Quasicrystalline metalic alloys are already used in a handful of commercial products, including as a coating for some non-stick frying pans because they combine the scratch- and temperature- resistant properties of a polymer such as Teflon with the heat conduction property of metals.

However, a major technical obstacle remains to using quasicrystal materials to minimize friction between surfaces sliding against one another, the scientists said. Microscopic surface contaminants, such as atmospheric gases, can come between the surfaces and interfere with the materials' high lubricity. The gases form a thin layer of molecules over the alloy surface-- typically in a crystalline pattern -- which masks the desirable surface properties of the underlying quasicrystal, they said.

The researchers' computer model of the effect of adsorbed gas on the quasicrystal alloy of aluminum, nickel and cobalt will be published in an upcoming issue of the journal Physical Review Letters. Their research was funded by the National Science Foundation.

"We are interested in quasicrystals because they are scratch-resistant and they have very little friction," said Stefano Curtarolo, lead author of the paper and a professor of materials science in Duke's Pratt School of Engineering. "So they are promising for sliding interfaces in machines and applications where the potential for scratching might be involved."

Metals were believed to have only periodic crystalline structures until 1984, when materials scientists reported discovery of the first metallic alloy with a quasicrystalline structure. Since then, scientists, including Curtarolo, have sought to explore the properties and applications of quasicrystals.

The challenge Curtarolo, Duke graduate student Wahyu Setyawan and their colleagues at Penn State University address in their paper is how to preserve the low-surface-friction property of a quasicrystal in the presence of a gas.

In previous experiments, Curtarolo's Penn State colleagues Nicola Ferralis, Renee D. Diehl, Raluca Trasca and Milton W. Cole had found that when xenon gas is exposed to their quasicrystal alloy, a single layer of xenon first forms in a quasicrystal pattern on top of the alloy, but by the time two or more layers formed, the xenon atoms develop a crystalline structure.

They chose to experiment with xenon, which does not react chemically with most metals, so they could consider the physical interaction of the gas and the metallic alloy, without complicating chemical interactions. In the experiments, the number of layers formed by the xenon atoms varies with the experimental temperature and pressure.

"If you have very little xenon gas, it's going to follow the aperiodic symmetry of the quasicrystal; if you have a lot, it's going to follow the periodic structure of xenon," Curtarolo said. "This change from quasicrystal to periodic crystal -- that's what we want to know about."

Cutarolo and his colleagues modeled in their computer simulation this transition from a single layer of xenon with quasicrystalline properties to multiple layers with crystalline properties. The simulation is consistent with experimental data.

The simulation is available online at nietzsche.mems.duke.edu/SCIENC … sotherm_T77K_big.mpg. In the simulation, the image on the left is of the average position of the xenon atom, the image on the right is of the electron diffraction pattern used to determine the position of the atoms and the graph on the bottom gives the density of the xenon gas.

"This model tells us how we might be able to control the transition and preserve the low-friction property of quasicrystals," Curtarolo said. "It's a step towards understanding how quasicrystals interact with gases in the atmosphere and how we could eventually use them in real machines."

Source: Duke University