THE STRAITS TIMES

Scientists develop AI to predict and engineer material properties

NTU president Professor Subra Suresh, a senior author of the study, said the new method made it possible to calculate the almost infinite number of potential combinations of material strain. PHOTO: SCIENCE JOURNAL

PUBLISHED 4 HOURS AGO

Scientists have developed a machine learning approach that can predict the effects of strain on the properties of materials, paving the way for new developments in communications, information processing and energy.

The research was done by Nanyang Technological University (NTU), together with the Massachusetts Institute of Technology (MIT) and Russia's Skolkovo Institute of Science and Technology.

When a semiconductor material is bent or strained, the atoms in its structure are perturbed, changing its properties such as how it conducts electricity, heat or light transmission.

NTU president Professor Subra Suresh, a senior author of the study, said the new method made it possible to calculate the almost infinite number of potential combinations of material strain. "Now we have this reasonably accurate method that drastically reduces the complexity of the calculations needed," he said.

"Our research is an illustration of how recent advances in seemingly distant fields such as material physics, artificial intelligence, computing and machine learning can be brought together to advance scientific knowledge that has strong implications for industry application."

In a paper published in the Proceedings of the National Academy of Sciences this week, the authors demonstrated their use of artificial intelligence to identify the most energy-efficient strain pathways that could transform diamond into more effective semiconductors.

Last year, the NTU and MIT authors reported in the journal Science that diamond nanoneedles could be bent and stretched as much as 9 per cent, which was surprising given that diamond is the hardest known natural material.

PUSHING THE LIMITS

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NTU PRESIDENT PROFESSOR SUBRA SURESH, describing the intersection of multiple scientific disciplines in the study.

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And in earlier research with industrial applications, "strain engineering" was used on silicon processor chips, where a one per cent strain allowed electrons to move faster, resulting in up to 50 per cent higher processing speeds.

In the latest study, the team examined the effects of strain on the bandgap, a key electronic property of semiconductors, in both silicon and diamond. Using their neural network algorithm, they predicted how different amounts and orientations of strain would affect the bandgap.

Being able to tune the bandgap could improve the efficiency of semiconductor materials such as a silicon solar cell, increasing the energy harnessed from light while making it a thousand times thinner, thus reducing the cost needed for materials, transportation and infrastructure, said NTU in a statement.

Diamond has shown great potential as a semiconductor material ideal for high-frequency devices such as radios in satellite communication and power electronics used for mobile networks and electrical power grids, it added.