Researchers create first exact model for diffusion in magnesium alloys

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The movement of atoms in solids controls everything.

In order to develop new materials, material engineers need to be able to predict how fast impurity atoms diffuse, or spread, in a crystal over a range of temperatures.

Using new computational techniques, researchers at the University of Illinois at Urbana-Champaign have constructed the first exact model for diffusion in magnesium alloys. While magnesium is the lightest structural metal, this new model could mean big things for material engineers, as it can also be used to predict how atoms diffuse in many other materials.

Einstein first described the fundamental mechanism of diffusion, but it has only been modeled exactly for a few crystals.

"Computer analysis of the magnesium crystal revealed hidden broken symmetries that impact how different atoms would move in magnesium," explained Dallas Trinkle, an associate professor of materials science and engineering at Illinois.

Combined with state-of-the-art quantum mechanics calculations, Trinkle and his PhD student Ravi Agarwal, were able to predict the diffusion of both common and rare earth metals, which can be used to further many vital, practical applications.

"Most substitutional solutes in solids diffuse via vacancies, however, widely used analytic models for diffusivity make uncontrolled approximations in the relations between atomic jump rates that reduce accuracy," said Agarwal, who is the first author of the study, "Exact Model of Vacancy-Mediated Solute Transport in Magnesium, published in *Physical Review Letters*. "Symmetry analysis of the hexagonal close packed crystal identifies more distinct vacancy transitions than prior models, and a Green function approach computes diffusivity exactly for solutes in magnesium. We found large differences for the solute drag of aluminum, zinc, and rare earth solutes, and improved diffusion activation energies—highlighting the need for exact analytic transport models."

"These new results will allow the creation of new, lightweight structural metals for automotive and aerospace applications," Trinkle said. "This model is particularly enlightening, as we are able to find broken symmetry in atomic moves that were previously thought to be identical. This method can now be used to predict how atoms diffuse in many other materials."

More information: Ravi Agarwal et al, Exact Model of Vacancy-Mediated Solute Transport in Magnesium, *Physical Review Letters* (2017). DOI: 10.1103/PhysRevLett.118.105901

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