Process for visualizing defects in crystal solids enhanced by artificial intelligence

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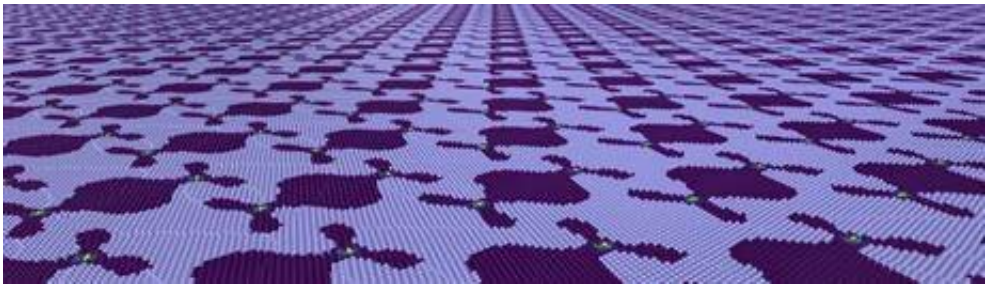

Credit: CEA

Crystals are ubiquitous: most metals, for example, are crystalline. Known for the almost perfect organization of their atoms, crystals nonetheless always contain imperfections, which are called defects. The concentration and morphology of defects in a crystalline solid have a direct influence on the properties of the material. Improving the understanding of crystal defects and their evolution will therefore make it easier to predict changes in how materials change over time. Understanding such changes is especially crucial for ensuring the optimal design of facilities subject to severe environmental conditions such as irradiation.

In modern materials science, researchers simulate the onset and evolution of defects in crystalline solids using very large-scale computer simulations. However, the immense stream of data generated makes

analyzing numerical simulation experiments an extremely complex process. Researchers at the CEA, the results of whose work have recently been published in *Nature Communications*, propose a novel approach that can be applied universally to overcome this difficulty. This new approach is the first method that can be applied to all materials with a crystalline structure. Providing a continuous visualization of a defect and its atomic environment, this facilitates the description of complex physical processes such as the migration of defects under irradiation.

The researchers, from the Nuclear Energy Division and the Military Applications Division of the CEA, have drawn on artificial intelligence methods to develop an algorithm that describes distortions in the local atomic environment caused by defects in the material. This distortion score facilitates automatic defect localization and enables a "stratified" description of defects that can be used to distinguish zones with different levels of distortion within the crystalline structure.

The results of this study open up many exciting possibilities for future development across the entire materials science community. These simulation tools can be used to automate analysis of huge datasets, such as those generated as a result of experimental techniques like atom probe tomography, transmission electron microscopy and synchrotron radiation , methods already being used to probe the mysteries of matter. These developments may also be applied in other fields, including chemistry, biology and medicine, for example, to detect cellular defects characteristic of cancer.

More information: Alexandra M. Goryaeva et al. Reinforcing materials modelling by encoding the structures of defects in crystalline solids into distortion scores, *Nature Communications* (2020). DOI: 10.1038/s41467-020-18282-2

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