Team offers new insights into radiation damage evolution

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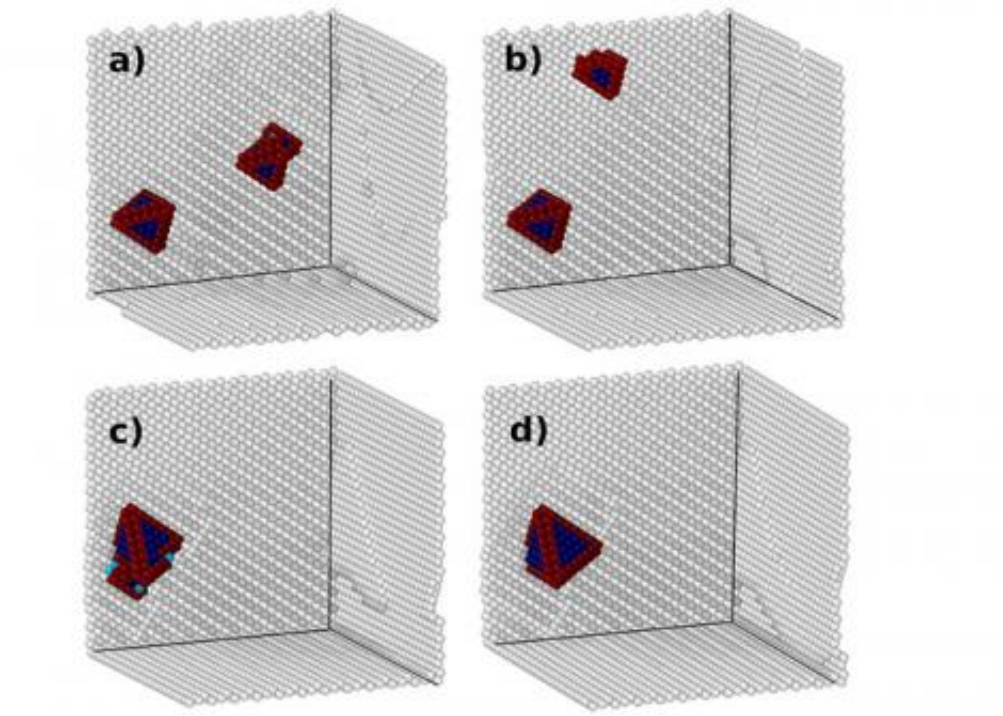

Researchers at Los Alamos are studying complex materials issues, in this case the defects deep inside certain types of cubic metals. This image shows a reaction between two "stacking fault tetrahedra," a perfect SFT containing 15 vacancies and a defective SFT containing 13 vacancies. As the smaller SFT migrates through the material, (frames a and b), it eventually encounters the larger SFT (frame c), reacting with it to form a larger, perfect SFT containing 28 vacancies. The time for this reaction to occur at 700 degrees K is 237.64 nanoseconds.

Two reports from Los Alamos National Laboratory this week in the *Nature* journal *Scientific Reports* are helping crack the code of how certain materials respond in the highly-damaging radiation environments within a nuclear reactor.

The goal of these efforts is to understand at an atomistic level just how materials develop defects during irradiation, and how those defects evolve to determine the ultimate fate of the material.

"The new insights provided by these studies will aid in both predicting and designing materials for improved performance and ultimately cost savings for nuclear energy production," said Blas Uberuaga, lead author of one of the reports.

Together, these results highlight the complex behavior of defects even in the simplest of materials. Further, "they provide insight into how defects evolve, properties that must be accounted for in predicting the performance of materials under irradiation," said Enrique Martinez Saez, lead author of the second report.

Go to "The relationship between grain boundary structure, defect mobility, and grain boundary sink efficiency," by Blas Pedro Uberuaga, Louis Vernon, Enrique Martinez Saez, and Arthur F. Voter.

Using long-time simulation methods, the Los Alamos researchers determined the mobility of defects and defect clusters at a variety of grain boundaries in copper. The work reveals key factors that could allow scientists to improve the functionality of nanocrystalline materials in extreme environments, such as nuclear reactors, where the interfaces are expected to promote radiation tolerance.

The researchers report that mobilities vary significantly with boundary structure and cluster size—the larger the cluster size, the less

mobility—and that interface-sink efficiency depends on kinetics of defects within the interface. Thus, sink efficiency is a strong function of defect mobility, which depends on boundary structure, a property that evolves with time. Further, defect mobility at boundaries can be slower than in the bulk, which has implications for the properties of polycrystalline materials more generally. The researchers used a combination of accelerated molecular dynamics, adaptive kinetic Monte Carlo, and object kinetic Monte Carlo to determine the mobility of defects at grain boundaries (GBs) and the impact on GB sink efficiency.

The new insight from these simulations indicates that the overall defect content in a nanocrystalline material is a competition of defect annihilation in the grain interiors and at the interfaces, which in turn is controlled by defect mobility within the interface, a property that depends on the interfacial character. Thus, the defect annihilation rate at the interfaces is a key property controlling the radiation tolerance in these materials. This work was supported by the US Department of Energy's Office of Basic Energy Sciences.

Go to "Mobility and coalescence of stacking fault tetrahedra in Cu," by Enrique Martinez Saez and Blas Pedro Uberuaga.

The second paper sheds light on discrepancies in the understanding of irradiated materials where, at temperatures above 500 K, only large voids are observed. These new insights into defect structures and their properties help interpret experimental observations that have not been explained previously.

The presence of stacking fault tetrahedra (SFTs) in materials dramatically modifies both the mechanical properties of the specimen and the evolution of the material under extreme environments. Understanding the evolution of such defects, especially growth mechanisms, is critical for predictive models of both the evolution and

subsequent properties of materials subjected to plastic deformation and irradiation. Current theory assumes that these defects, once created, are static objects.

Using molecular dynamics and temperature accelerated dynamics simulations to study a simple metal, fcc copper, the Los Alamos researchers show that, counter to conventional wisdom, SFTs can exhibit extremely high mobilities, even higher than single vacancies.

The large mobility of defected SFTs provides a possible explanation for the dearth of small SFTs at the high temperature regime (above 500 K) observed experimentally. This study proposes a new growth mechanism for SFTs by which small SFTs interact with one another to form larger ones. This work demonstrates that SFT mobility itself might be a critical mass transfer mechanism in the evolution of cold-worked or radiation-damaged materials that must be accounted for in larger scale models to make accurate predictions.

Provided by Los Alamos National Laboratory