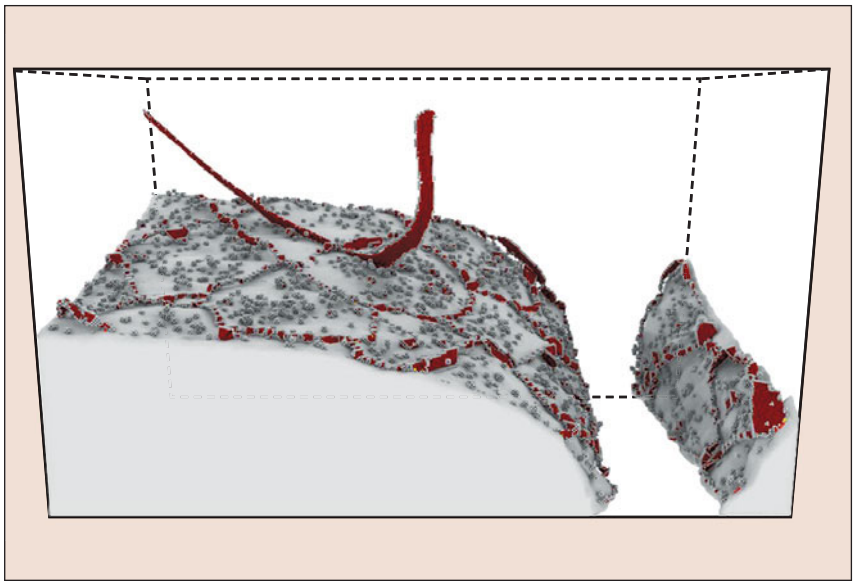
Realistic simulations reveal atomic-scale details responsible for superalloy properties

A recent study of nickel-aluminum superalloys has given researchers their first glimpse of the atomic-scale details responsible for the phenomenal properties of superalloys. By performing molecular dynamics simulations based on realistic, experimentally informed structures, the researchers were able to observe the interactions of defects and precipitate phases in nickel-aluminum superalloys under stress. The results will help inform efforts to make increasingly high-temperature superalloys with less dependence on strategic elements like rhenium.

Superalloys are of tremendous industrial importance. Found in the blades of all gas turbines for airplane engines and power plants, single crystal nickel-base superalloys provide excellent mechanical strength and stability at high temperatures. In these materials, precipitate impurity phases impede the movement of dislocation defects, which tend to be responsible for plasticity. These interactions have not yet been observed experimentally, however, which fundamentally limits an understanding of superalloys and hinders the ability to engineer ever-greater superalloys.

Now, a team of researchers have illuminated some of the critical atomic-scale details of superalloys through atomistic simulations. The team, hailing from Friedrich-Alexander-Universität Erlangen-Nürnberg, The Ohio State University, and the Max-Planck-Institut für Eisenforschung, published their findings in the June 15 issue of *Acta Materialia* (DOI: 10.1016/j.actamat.2015.03.050; p. 33).

"This was the first time someone has taken experimental microstructures, put them in a computer, and simulated what happens in this process of dislocation/precipitate interaction, which is one of the most important strengthening mechanisms in these superalloys," says Erik Bitzek, lead author of the study. "We did all this at high temperatures and could directly observe a lot of processes which had been postulated before on the basis of individual post-mortem [transmission electron] micrographs," says Bitzek.



Superalloy simulations provide an unprecedented view into the interactions of dislocations and precipitates in these technologically critical materials. Credit: *Acta Materialia*.

Up until now, simulations have been limited to quasi-two dimensions with idealized configurations. These have yielded insight and valuable quantitative information, but the studies are fundamentally limited. Here, the researchers made two important advances: simulating the system in three dimensions, and starting from realistic structures determined through atom probe tomography.

Bitzek and colleagues initiated their simulations with morphologies acquired through atom probe tomography of superalloy specimens that were first subjected to heat cycles to simulate aging. From these data, the researchers extracted information about the boundaries between the matrix phase (γ) and the precipitate phase (γ'). Having determined the shape and location of those boundaries, the researchers then filled in the atomic positions in the simulation. From this starting configuration, consisting of 14 million atoms, they then performed molecular dynamics simulations, inserting dislocations and applying shear stresses to explore the system's response.

"Our main finding was that the local curvature of the precipitate influences the misfit dislocation network," says Bitzek; "If you had a totally planar interface, you'd get a different dislocation network and different interactions. It was really exciting to see that the dislocations in our network actually exhibited the same core structure as seen in the experiments."

The team also witnessed the atomic-scale details of mechanisms previously proposed but never observed, such as "knitting out" dislocations from misfit-dislocation networks through collinear interactions between two dislocations. This mechanism helps prevent dislocations from cutting into the matrix phase, which would weaken the material. This type of interaction cannot be produced in quasi-two-dimensional simulations with idealized structures, underscoring the importance of working in three dimensions.

Examples of the behaviors found in these simulations are showcased in a video produced by the researchers: https://www.youtube.com/watch?v=K7fEZURZhkA.

The research team plans to make their simulation code, *nanoSCULPT*, freely available for other researchers to use.

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