Strategic control of atomic-scale defects for tuning properties in metals

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Advanced metallic alloys can benefit from clusters of dopant atoms and intermetallic particles to improve their performance. Suhas Eswarappa Prameela, Peng Yi, Michael Falk and Tim Weihs discuss how atomic-scale defects can be used to form these clusters and particles.

Metals are useful in almost every industry, from microelectronics to large-scale infrastructure. The demand for improved performance has led researchers to continue to design stronger, lighter, more functional and less expensive metallic alloys by altering processing or chemistry. Research on crystalline metals has been dominated for decades by the study of defects inherent in them, including vacancies, dislocations, twins and grain boundaries, which dictate how the metals perform. The role of atomic scale defects in the mechanical failure of metals has been a significant area of interest for this field. Although deviations from crystalline order are called 'defects,' implying that they are generally detrimental to properties, such features can often be leveraged during processing to improve the metal's performance. It is now possible to artificially inject atomic-scale defects strategically to tune the properties of metals in an unprecedented manner by helping to aggregate dopant atoms, thereby facilitating their impact.

A common method to improve the performance of a metal is to alloy it with a small concentration of other metals (dopants or solutes). This process often involves aging or heat-treating the alloys to induce phase transformations in which large ensembles of solute and parent metal atoms combine to form intermetallic particles with a specific stoichiometry. The resulting particles are often referred to as precipitates and can inhibit the motion of dislocations, thereby strengthening the metallic alloys. However, traditional aging can be time-consuming (running to several days) and inefficient. To overcome this problem, one can facilitate the nucleation of precipitates using atomic-scale defects.

Common atomic-scale defects in metals are vacancies (unoccupied sites in the crystal lattice) and line defects such as dislocations (edges of shifted planes of atoms) that nucleate and glide when the metal is permanently deformed (FIG. 1a). Because these defects cause local atomic disturbances, they generate local stress fields (FIG. 1b) that often dominate their interaction with other defects, such as neighboring dislocation lines or solute atoms. For example, in the edge dislocation shown in FIG. 1a, atoms above the dislocation are squeezed together, resulting in a compressive stress field. Conversely, atoms below the dislocation experience a tensile stress field.

The stress field near a dislocation attracts vacancies and/or solute atoms, because their presence above or below the dislocation can reduce local stresses, thereby decreasing local elastic strain energy. This attraction can produce solute clusters near the dislocation core (FIG. 1c), which can form precipitates more rapidly than in traditional aging processes, leading to a higher number density of precipitates in far less time. The rapid diffusion of solute atoms along the dislocation lines can also accelerate this process.

Short segments of dislocations called jogs can produce vacancies as they move within the lattice. The vacancies have high mobility, hopping one atomic site at a time, and lead to faster atomic diffusion that speeds solute clustering and precipitation in metallic alloys. This has been shown for aluminum alloys in cases where cyclic straining produces vacancies that in turn promote a higher density of solute clusters and fine precipitates[1]. The high density of clusters and precipitates boosts the mechanical strength of the alloys dramatically. Better yet, this process can be turned off rapidly as needed. Given that vacancies have a relatively short lifetime, stopping the cyclic straining results in the annihilation of vacancies, a reduction in solute transport and far slower clustering and precipitation.

Beyond enabling clustering of solute atoms, vacancies can also cluster themselves to form voids, which are often seen in metals under irradiation. Free surfaces and local stress concentrations near vacancy clusters may provide additional driving forces for solute segregation. Beyond dislocations and vacancies, solutes can also segregate to planar interfaces between crystals or twinned regions common to polycrystalline metals. Altering the nature of these interfaces with a periodic array of solute atoms[2] and precipitates can significantly improve mechanical and electrical properties.

There are several examples where defect-assisted solute segregation has been used to improve the properties of metals. Atomic-resolution, high-angle annular dark-field (HAADF) scanning transmission electron

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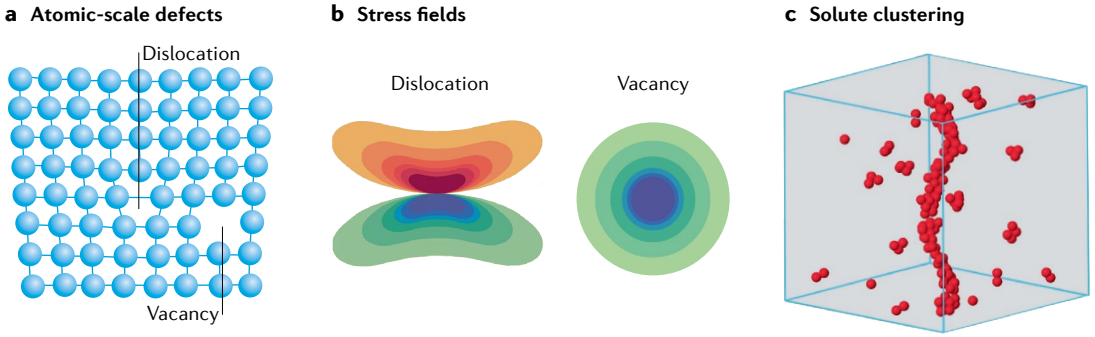

Fig. 1 | **Atomic-scale defects. a** | A dislocation and a vacancy in a 2D square lattice. **b** | Stress fields around an edge dislocation and vacancy of a single atom. **c** | Solute clustering near and far from a dislocation line. Image courtesy of Stephanie Hernandez, Johns Hopkins University.

microscopy showed substantial lattice strain near dislocation cores in magnesium–zinc alloys and the subsequent segregation of zinc atoms[3]. Similar success was achieved in magnesium–aluminium alloys, in which aluminium atoms segregated to dislocation cores and yielded nanoscale precipitates with improved mechanical properties[4]. Given that magnesium alloys are ~35% less dense than aluminium alloys, incorporating such clusters and precipitates can substantially boost critical properties such as specific yield or fracture strength[5]. In addition to light metals, alloys of nickel, titanium and iron also demonstrate this phenomenon. For example, linear complexions (stable chemical and structural solute phases confined at line defects) in an iron–manganese alloy have been reported, providing more significant insights into nano-structuring of metallic alloys[6]. Injecting dislocations offers a template for controlling the motion and impact of solute atoms. Beyond mechanical strength, newly formed solute segregates have been found to alter magnetic states in iron alloys, providing a pathway to tune the magnetic properties of materials.

Advances in experimental characterization techniques and powerful computational tools are providing a deeper understanding of these complex, non-equilibrium phenomena with improved spatial and temporal resolutions. Experimental techniques such as atom probe tomography[6,7], transmission electron microscopy[1,4] and field ion microscopy[8] now offer near-atomic scale images of defects coupled with the chemical mapping of solute atoms. For example, individual rhenium atoms near defects in nickel alloys have been imaged[8]. These techniques offer direct imaging of dislocation cores and their surrounding lattice distortions, and they can be coupled with density functional theory calculations, molecular dynamics and dislocation dynamics simulations that mimic the local conditions to predict the pressures, stresses, clustering and precipitation. Such tools are crucial for observing and understanding the segregation of solute atoms to defects. Understanding how these defects behave can help control the distributions of solute atoms, leading to a bottom-up approach for designing advanced materials. For example, it has been argued that understanding the role of defects and solute clusters can enhance the development of fusion materials for nuclear applications[9]. Furthermore, machine learning methods can be used with the resulting data on defects and solute atoms to more effectively tune material properties in new ways[10]. With such tools, it is possible to optimize the deployment of atomic-scale defects to yield superior metallic materials. In addition, the concepts and methods could also benefit the design of non-traditional materials such as high entropy alloys.

Aided by these experimental advancements, developing multiscale computation models for predictive processing design is a promising direction. However, challenges remain on computational and theoretical levels. For example, simulation techniques, including physically well-grounded acceleration algorithms and robust multi-scale simulation schemes, are needed to develop and test atomic-scale theories capable of predicting the effects of advanced processing. Achieving such high-fidelity simulation requires a more in-depth study of the statistical physics of non-equilibrium processes. Physicists will need to think more deeply about how we might understand the behavior of heavily defected materials that are so far from the perfect crystalline state that one can no longer consider isolated defects as adequate building blocks for predictive theories.

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Competing interests
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