Playing with defects in metals

Xiuyan Li and **K. Lu** discuss a strategy, alternative to alloying, to tailor the mechanical properties of metals. By engineering defects, metals with bespoke performance might be obtained while reducing the materials' compositional complexity.

For centuries, the development of structural metals has primarily relied on the art of alloying: combining a metal with other elements to obtain desired properties. Such processes aim to change the electronic and strain energy states of the lattice, so that its properties are modified, or form alternative phases with completely different properties. For example, alloying iron with chromium and nickel leads the formation of a layer that protects the material from oxidation and corrosion. Alloying iron with carbon produces harder ferrite and/or carbide compounds, or induces the transformation to a martensitic phase that is harder to deform. A broad tunability of the microstructural (and, consequently, mechanical) properties has been demonstrated by adjusting the alloy composition with the addition of an increasing number of elements — for instance, as many as ten different elements are now included in the nominal composition of state-of-the-art aerospace superalloys[1].

However, such a strategy may have a negative impact on the long-term sustainability of high-performing metals. Alloying makes materials development more resource-dependent, exposing it to the risks associated with progressive resource exhaustion and unavailability of critical elements. Moreover, alloyed materials with complicated compositions may become more difficult to recycle — in fact, it has been reported that the majority of alloying metals and metalloids in the periodical table are either non-recyclable or scarcely recycled[2]. In addition, the overall production costs increase progressively with alloying, especially for those materials that include precious elements. For instance, adding 1% rhenium in superalloys improves mechanical performance, but can double the total material cost. Hence, although the advantages of alloying in terms of properties are clear, special attention has to be taken to control the potential increases in costs and environmental burden related to this engineering strategy.

Various imperfections or defects in crystalline materials, such as vacancies, dislocations, and grain or phase boundaries, can also substantially change material properties. A familiar example of such an effect is the work-hardening of iron due to an increased number of dislocations and grain boundaries, generated when it is repeatedly bent back and forth. The imperfections could apparently act as alloying elements for tuning properties without changing chemical compositions. However, the widespread use of imperfections for materials development is limited by their instability. On mechanical or thermal loading during processing or in service, these imperfections become mobile and interact with each other, resulting in annihilation or transformation from one type to another — the effect of iron work-hardening, for instance, is lost if the material is exposed to a thermal annealing process. Moreover, the generation of defects under ordinary processing conditions is limited and challenging to control — for example, plastic deformation inducing processes like rolling or drawing may introduce grain boundaries into metals and refine grains, yet in most metals this refinement saturates at the submicrometre scale due to grain boundary annihilation above a threshold level of strain[3].

In the past few decades, significant progress has been made in stabilizing metal imperfections and in manipulating interfaces at different length scales, resulting in substantial tuning of the mechanical properties and their combination[4]. Several types of low-energy interfaces, including twin boundaries and low-angle boundaries, exhibit rather high stability against thermal and mechanical stimuli at the nanoscale. This has been used to simultaneously obtain ultrahigh hardness and thermal stability — which are usually mutually exclusive in conventional materials — in nickel with nanolaminated structures containing high-density low-angle grain boundaries[4]. Engineering of nanotwinned structures

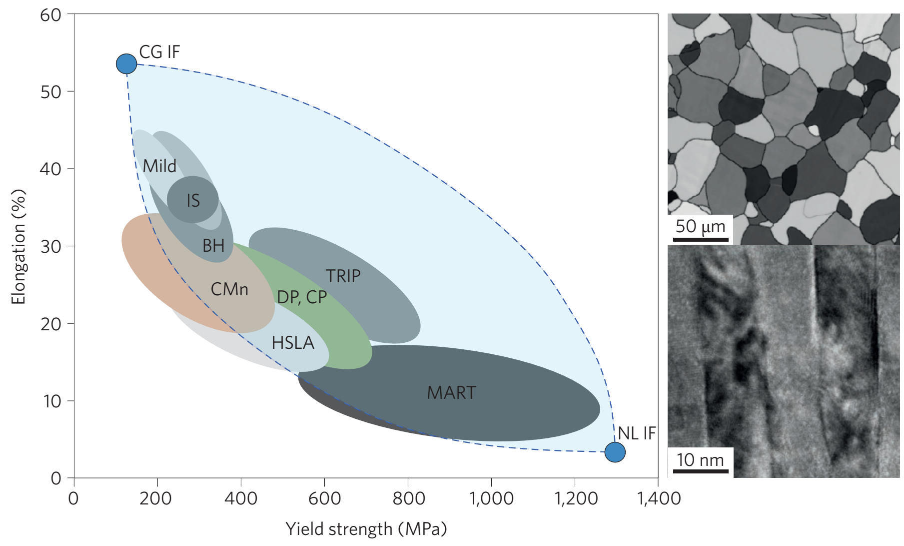

Figure 1 | A range of mechanical properties that can be obtained by engineering defects in metals. Strength–ductility correlations for different types of steels. IS, isotropic; BH, bake-hardening; CMn, carbon-magnesium; HSLA, high-strength–low-alloyed; DP, dual-phase; CP, complex-phase; TRIP, transformation-induced plasticity; MART, martensitic; IF, interstitial-free. Coarse-grained (CG) IF steels (a scanning electron microscopy image of their morphology is shown in the top right) are soft and ductile. Nanolaminated (NL) IF steels (a transmission electron microscopy image[9] of this morphology is shown in the bottom right) are very hard but less ductile. Gradient nanostructures combining these two extreme morphologies provide a broad range of strength–ductility combinations as outlined by the dashed lines. X.C. Liu is acknowledged for support in preparing the figure. Adapted from ref. 10, Wiley (graph); and ref. 9, Elsevier (right images).

enables the synthesis of materials that combine various interesting properties[5], such as ultrahigh strength with high electrical conductivity, or high strength with ductility and thermal stability[6]. Interfaces can also be stabilized by structural relaxation and segregation of solute atoms, which facilitates structural refinement down to the nanoscale[7].

Controlling the distribution and organization of defects offers another degree of freedom for the engineering of material properties. For instance, gradient distribution of interfaces with spacing ranging from the nano- to the macroscale is an effective strategy for strain delocalization[4], resulting in remarkable enhancements in fatigue resistance and reduction of friction coefficient and wear rates[8]. Using this gradient approach, the mechanical properties of steel with a fixed chemical composition can be tuned across several length scales, spanning the performance of multiple steels engineered through alloying and other approaches (Fig. 1). This example demonstrates that proper manipulation of structure, quantity and distribution of imperfections may allow a reduced number of materials to fulfil a broad range of mechanical specifications required for the realization of advanced devices and applications.

From a sustainability viewpoint, the development of high-performing metals with less or no alloying would make them less dependent on the availability of critical resources. The reduced number of materials used may also facilitate separation and sorting at the end of life, which constitute a considerable part of the total cost of recycling. Of course, in order to quantitatively assess the possible benefits of this approach, further studies on the performance stability during real-life applications and a detailed assessment of the environmental and economic impact of replacing alloyed metals with defect-engineered ones will be required.

It is also worth mentioning that this materials design approach will require proper adaptation of materials processing and manufacturing at the industrial scale. In conventional manufacturing, materials are processed to desired properties prior to shaping and component assembly. With this alternative approach, properties can be adjusted after the materials are shaped, with the added possibility of further manipulating the imperfections locally to impart specific mechanical behaviours at different points in the component. The modification of well-established metal manufacturing processes is, however, not a trivial task, and it can only take place once the technological advantages of this strategy, as well as its robustness against extreme processing and usage conditions, are demonstrated. Furthermore, fundamental understanding of the nature of the imperfections, and their stabilization and manipulation at different length scales is necessary to reach this goal. More efficient solutions could possibly be obtained by combining this defect-engineering strategy with some of the traditional alloying principles used today, while keeping the number of elements incorporated into an alloy limited. Finally, a major impulse to this manufacturing shift will be provided if full life-cycle assessment demonstrates reduced environmental burden and improved long-term sustainability. ❐

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