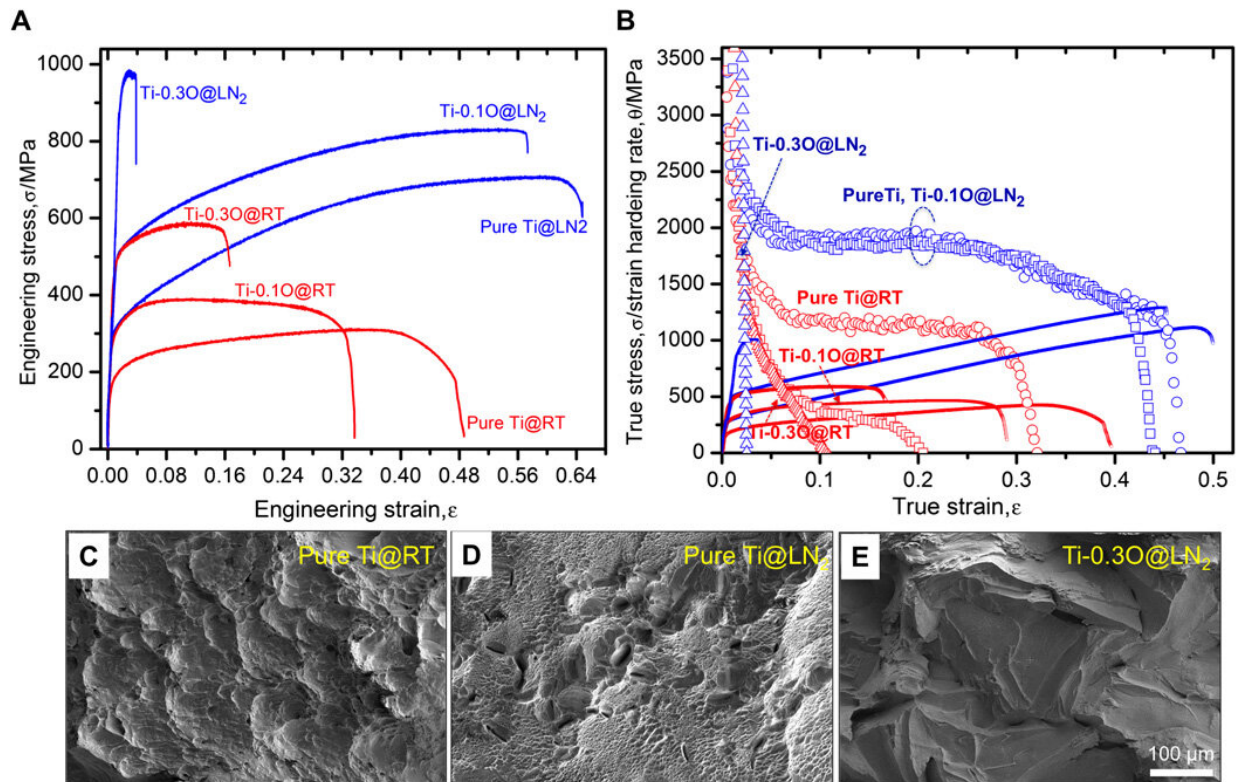


Mechanistic basis of oxygen sensitivity in titanium

October 30 2020, by Thamarasee Jeewandara



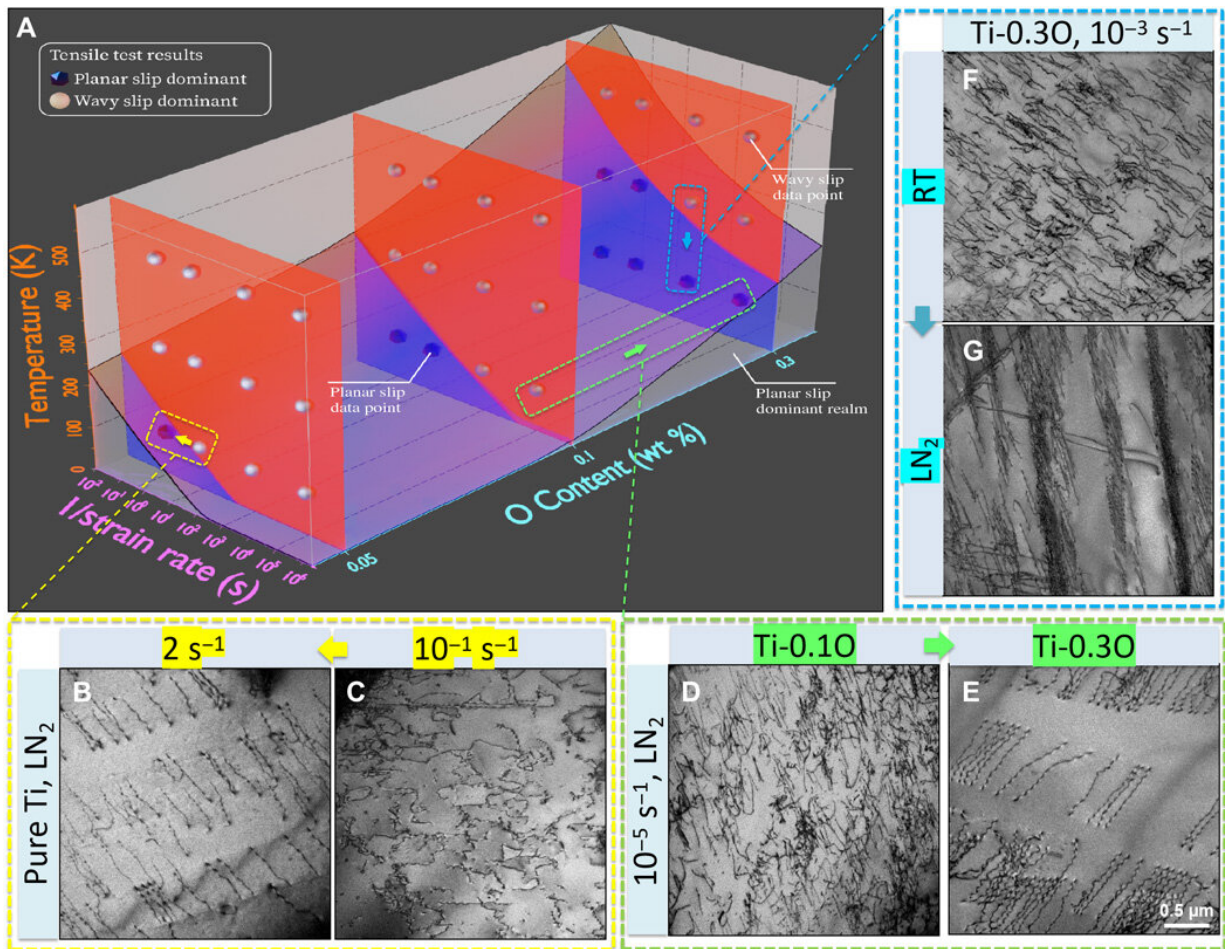
Mechanical behaviors of pure Ti, Ti-0.1O, and Ti-0.3O alloys at room temperature (RT) (~ 300 K) and cryogenic temperature (~ 100 K). (A) Representative engineering stress-strain curves of the three alloys with a strain rate of 10^{-3} s $^{-1}$. (B) Corresponding true stress-true strain curves (solid lines) and strain hardening rate (symbols) curves of the three alloys. (C) Fracture tomography of pure Ti at room temperature. (D) Fracture tomography of pure Ti at cryogenic temperature. (E) Fracture tomography of Ti-0.3O at cryogenic temperature. Credit: Science Advances, doi: 10.1126/sciadv.abc4060

Titanium is extremely sensitive to small amounts of oxygen, which can lead to markedly decreased ductility of the material. Materials scientists therefore aim to lower the costs of purifying titanium, while avoiding the poisoning effects of oxygen. In a new report now on *Science Advances*, Yan Chong, and a team of scientists in materials science and engineering at the University of California Berkeley and the Lawrence Berkeley National Laboratory in the U.S., detailed a systematic study on oxygen sensitivity of titanium. The team provided a clear mechanistic view of the effects of oxygen impurities on the mechanical properties of the material. The experimental and computational work provided insights for a rationale to design titanium alloys with increased tolerance to the variations in interstitial content (a position between the regular positions in an array of atoms in a material), with notable implications to facilitate the widespread use of titanium alloys in spacecrafts, naval ships, aircrafts and materials engineering.

Titanium alloys

Titanium alloys contain highly desirable properties including corrosion resistance and high specific strength making them attractive structural materials across a wide range of commercial applications. Interstitial atoms can be intentionally or naturally [incorporated to influence](#) the mechanical properties of titanium. Oxygen is a predominant interstitial impurity, widely adopted in titanium-based alloys to enable a potent strengthening effect [for diverse applications](#). Titanium is also inherently expensive due to the tight control of interstitial impurities during their manufacture. Although researchers have documented the [embrittlement effects](#) of interstitial impurities in [alpha-titanium](#) alloys, the mechanistic origin of the anomalous oxygen sensitivity on the mechanical properties remain to be understood, thereby limiting alloy design and processing strategies. Materials scientists had documented [a "wavy-to-planar" transition](#) of dislocation arrangements with increasing oxygen content in the metal. In the present work, Chong et al. conducted a systematic

multiscale investigation of the mechanical properties and deformation microstructures of titanium.



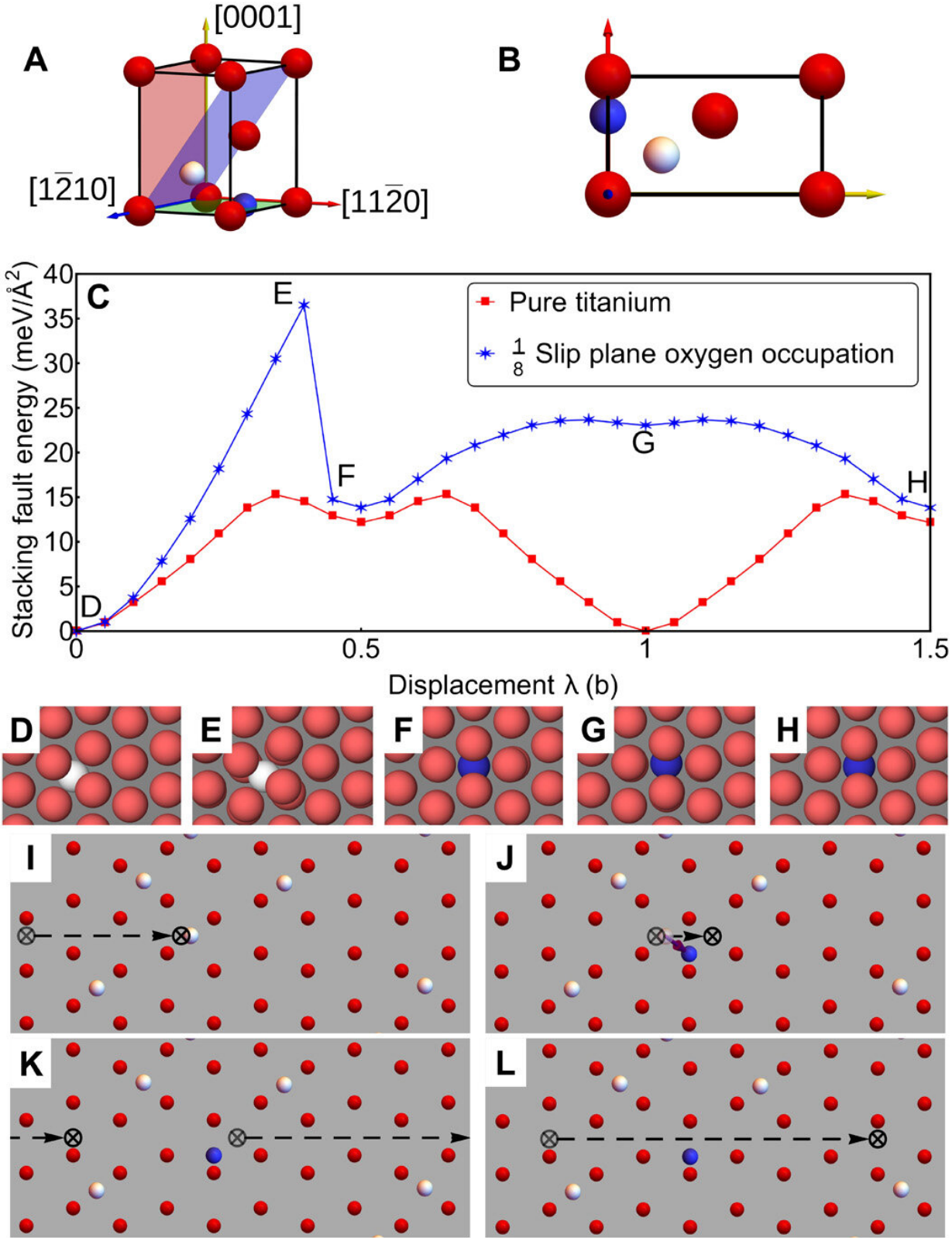
Comparison of typical dislocation morphologies (wavy or planar slip dominant) in Ti-O alloys after interrupted tensile deformations at different temperatures (500, 300, and 100 K) and strain rates (10^{-5}s^{-1} , 10^{-3}s^{-1} , 10^{-1}s^{-1} , and 2s^{-1}). The tensile strain was 4.0% for all the microstructures. (A) 3D diagram demonstrating the combined analysis of temperature, strain rate, and oxygen content dependences of dislocation morphologies in Ti-O alloys. A general tendency of wavy-to-planar slip transition occurred with either increasing strain rate, i.e., from (C) (pure Ti, 10^{-1}s^{-1} , LN₂) to (B) (pure Ti, 2s^{-1} , LN₂), or increasing oxygen content, i.e., from (D) (Ti-0.10, 10^{-5}s^{-1} , LN₂) to (E) (Ti-0.30, 10^{-5}s^{-1} , LN₂), or decreasing temperature, i.e., from (F) (Ti-0.30,

10^{-3} s^{-1} , RT) to (G) (Ti-0.3O, 10^{-3} s^{-1} , LN2). The transition boundary delineating wavy slip–dominant and planar slip–dominant regions gradually shifted toward a higher temperature and lower strain rate direction with increasing oxygen content. Credit: Science Advances, doi: 10.1126/sciadv.abc4060

The influence of oxygen on the mechanical properties of titanium alloys

The team aimed to reveal the nature of slip polarity associated with higher oxygen content relative to interstitial concentration, strain rate and deformation temperatures. They credited the marked oxygen sensitivity in titanium to transitions in dislocation behavior and [twinning activity](#) of the metal. The scientists discussed the atomic origin of the transitions relative to [density functional theory](#) (DFT) and [molecular dynamics](#) (MD) simulations to provide deeper insights to design interstitial-tolerant titanium alloys. Chong et al. tested three model alloys including pure titanium (with 0.05 weight percentage or wt %), Ti-0.10 (with 0.10 weight percentage—wt%) and Ti-0.30 (with 0.30 wt%) at high temperature, room temperature and cryogenic temperatures using [uniaxial tensile tests](#). A slight variation of the oxygen content caused marked changes to the mechanical properties of Ti-O alloys at room temperature and cryogenic temperatures. The observed failures of Ti-0.30 alloys at low temperatures highlighted its limitations for applications at cryogenic conditions. The strain hardening potential of the Ti-O alloys decreased with increasing oxygen content. Pure Ti and Ti-0.10 exhibited excellent and almost identical strain-hardening rates at cryogenic temperature.

Dislocation activity



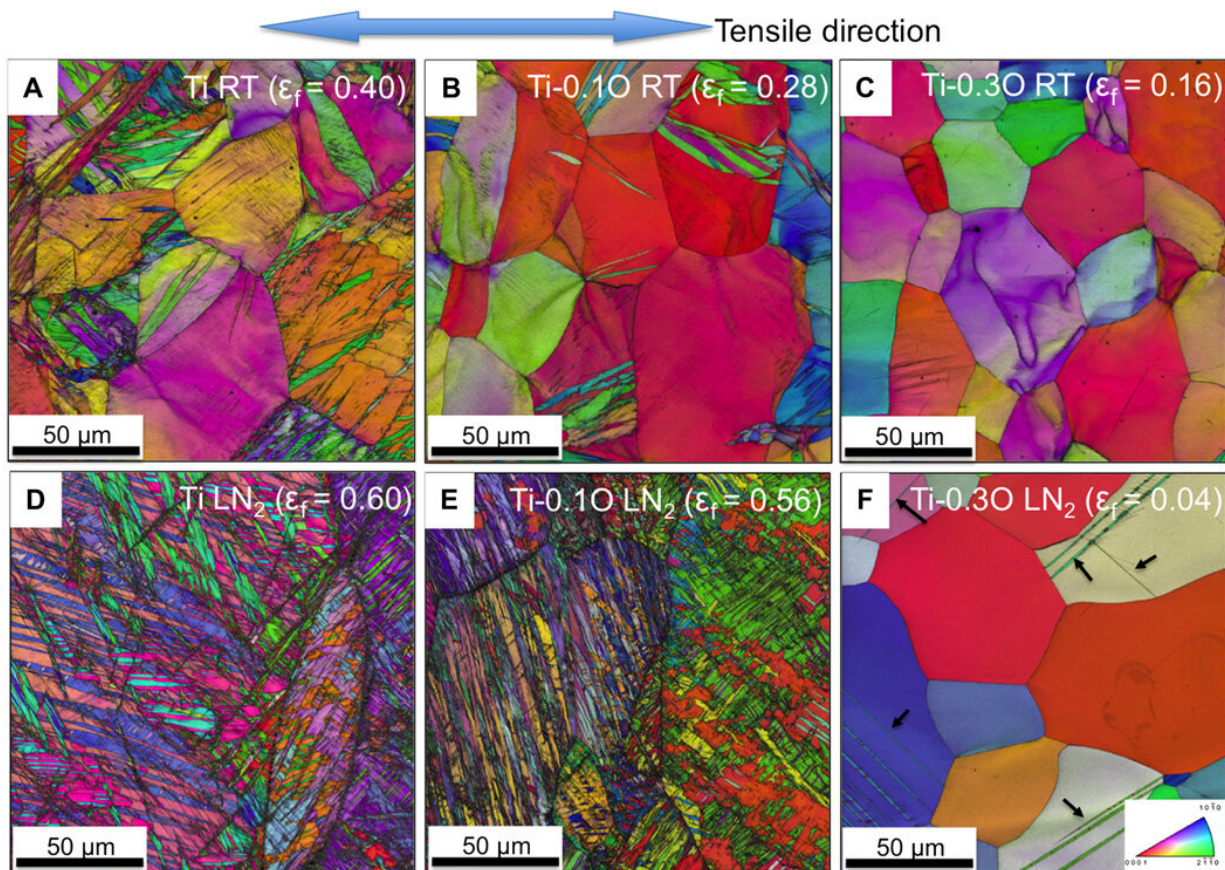
Schematic illustration of ISM of slip plane softening. (A) HCP lattice with octahedral (white) and hexahedral (blue) sites, and prismatic, pyramidal, and basal planes (red, blue, and green). (B) Orientation for the steps of dislocation slip shown in (I) to (L). (C) Modified GSF energy on the prismatic plane calculated with DFT. (D) to (H) show oxygen position for selected steps, starting from octahedral (D). (E) shows the distorted octahedral site at the maximum in energy. In steps (F) and (H), the oxygen is in an octahedral site formed at the stacking fault. (G) shows the hexahedral site. (I) to (L) demonstrate the key steps in the ISM model. In (I), the first dislocation (cross symbol) on a prismatic plane encounters an octahedral oxygen and slip is resisted. It eventually overcomes this obstacle and shuffles the oxygen to the hexahedral site (J). The dislocation continues slipping, and subsequent dislocations follow behind (K). These dislocations see a reduced barrier from the hexahedral oxygen and thus easily slip on this plane (L). Credit: Science Advances, doi: 10.1126/sciadv.abc4060

Chong et al. then investigated the typical dislocation morphologies of Ti-O alloys either in a wavy or planar slip-dominant mode through interrupted tensile deformations at different temperatures and strain rates. They schematically combined the analyses of temperature, strain rate and oxygen content dependence of the dislocation morphology. Using [transmission electron microscopy](#) (TEM) the team examined the representative dislocation morphologies relative to strain rate, oxygen concentration and deformation temperature. They noted the susceptibility for a wavy-to-planar slip transition (displacement of one part of the crystallographic plane of the material relative to another plane and direction) to occur when the strain rate or the oxygen rate increased, or with decreasing temperature.

Although the planar slip was [frequently reported](#) in Ti-O alloys at cryogenic temperatures, the underlying mechanism remains unknown. The [short-range-ordering](#) (SRO) or the regular and predictable arrangement of atoms across a short distance, for oxygen atoms, could

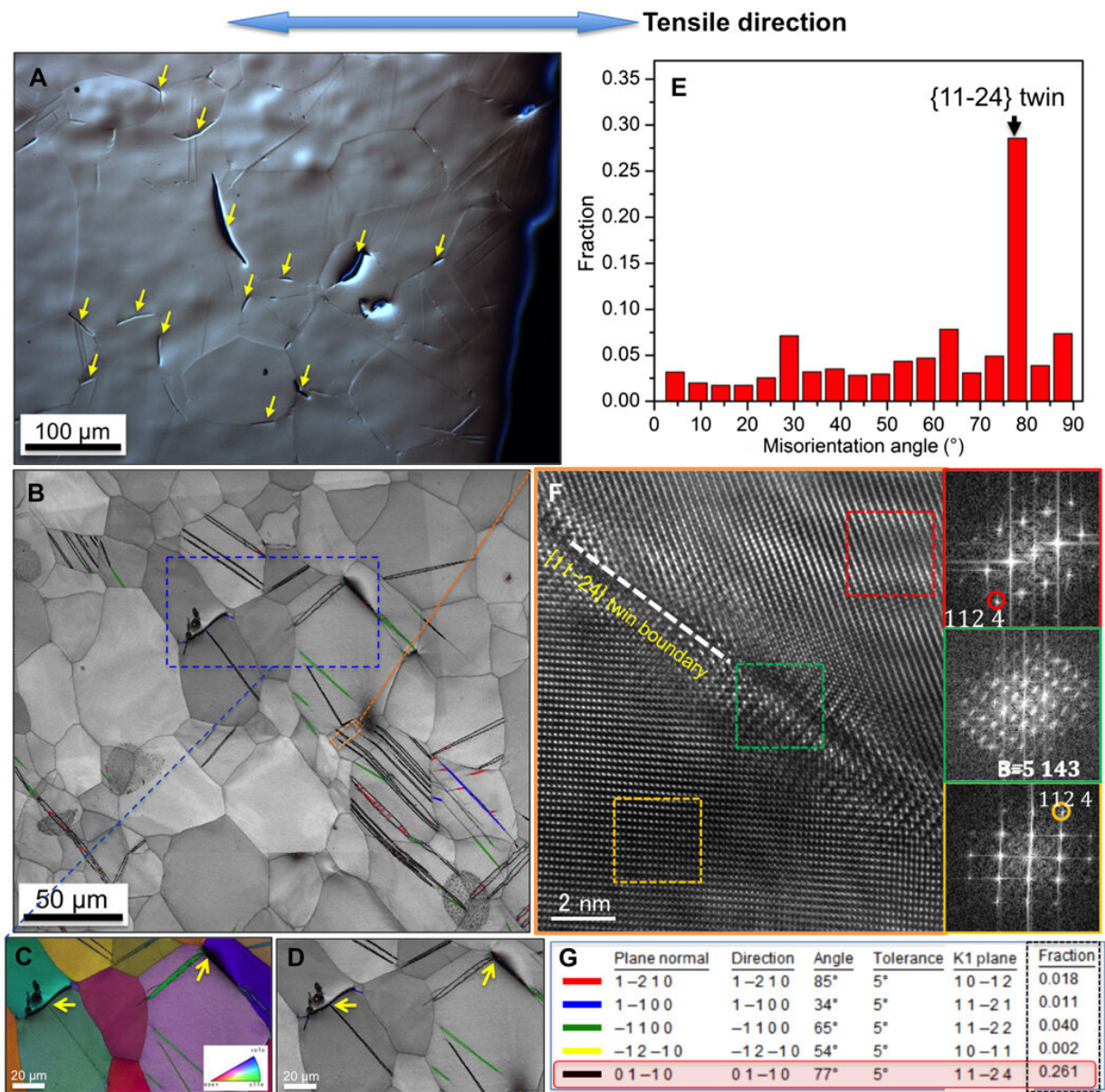
be a proposed mechanism; however, researchers have not yet experimentally verified the SRO of oxygen in the Ti-O binary system with a dilute oxygen content. The team therefore calculated the [diffuse antiphase boundary](#) (DAPB) energies and confirmed planar slip to be temperature and strain independent for [titanium-aluminide \(Ti-Al\)-based](#) alloys, in marked contrast to Ti-O alloys whose planar slip depended on the temperature and strain. The scientists therefore deduced a different origin to the evolving planar slip in Ti-O alloys.

Interstitial shuffling in the Ti-O system and deformation twinning



Inverse pole figure (IPF) + image quality (IQ) maps of Ti-O alloys after tensile

fractured at room temperature (RT) and cryogenic temperature (LN2), with a strain rate of 10^{-3} s $^{-1}$. (A) Pure Ti, RT, and fracture strain: 0.40. (B) Ti-0.10, RT, and fracture strain: 0.28. (C) Ti-0.30, RT, and fracture strain: 0.16. (D) Pure Ti, LN2, and fracture strain: 0.60. (E) Ti-0.10, LN2, and fracture strain: 0.56. (F) Ti-0.30, LN2, and fracture strain: 0.04. The tensile direction is horizontal for all the microstructures. Credit: Science Advances, doi: 10.1126/sciadv.abc4060



Characterization of Ti-0.3O alloy after tensile fractured at cryogenic temperature. (A) Optical microscopy of the area near fracture surface, in which several microcracks (as indicated by yellow arrows) were observed along the grain boundaries. (B) Twin boundary map showing the types of twins near the fracture surface [according to the colors shown in (G)]. (C) and (D) are the IPF map and twin boundary map showing one typical example of microcracks forming at the points where $\{11-24\}$ twins were blocked at the grain boundaries. (E) The misorientation angle profile, in which an evident peak was found at 77° , confirming the predominance of $\{11-24\}$ twins in Ti-0.3O deformed at cryogenic temperature. (F) The HRTEM image (from a zone axis of $[-5143]$) of one $\{11-24\}$ twin lifted out from the rectangle area in (B) by the focused ion beam (FIB) method. (G) The colors used in panels B and D. Credit: Science Advances, doi: 10.1126/sciadv.abc4060

Chong et al. conducted DFT (density functional theory) calculations to propose interstitial shuffling mechanisms (ISM) for the temperature and rate dependence of wavy-to-planar slip transitions in Ti-O alloys. Based on [generalized stacking fault](#) (GSF) energies obtained via computational calculations, the team provided evidence for the slip plane softening effect associated with the shuffling process in the material at lower temperatures and larger strain rates. The oxygen atoms that displaced within the material during the deformation process remained in their positions, reducing the barrier to further slip. The concept of [twinning](#) can also give rise to excellent mechanical properties of titanium alloys observed at cryogenic temperatures where dislocation activities typically become difficult.

Researchers have to date reported four [common deformation twinning modes](#) in titanium, including two tension twins (T1 and T2) and two compression twins (C1 and C2). Chong et al. considered an overview of twinning behavior as a function of oxygen content and temperature.

With increasing oxygen content, the twin fractions at room temperature were continuously reduced to the point where no appreciable twins could be detected in Ti-0.30 alloys at room temperature. The twinning activity enhanced substantially in pure titanium at cryogenic temperatures. They credited the enhanced feature in pure titanium to a larger internal stress level. To further understand the anomalous behavior of twins, the scientists studied the interactions between oxygen and twin boundaries using atomic simulations.

Outlook

In this way, Yan Chong and colleagues considered the systematic influence of oxygen on the dislocation morphology and twinning fraction to present a mechanistic view of oxygen sensitivity on the mechanical properties of titanium. They credited the origin of temperature strain rate and oxygen content sensitivity of Ti-O alloy slip planarity to the motion of [oxygen](#) atoms instead of short-range ordering of atoms. The model of interstitial shuffling mechanisms (ISM) provided an explanation to the observed [temperature](#) and strain sensitivity of planar slip in Ti-O alloys. The simulated alloy design strategies that interrupted the interstitial shuffling process in this work may notably increase the interstitial tolerance of [titanium alloys](#) to offer strengthening effects without an accompanying sacrifice in ductility.

More information: Yan Chong et al. Mechanistic basis of oxygen sensitivity in titanium, *Science Advances* (2020). [DOI: 10.1126/sciadv.abc4060](#)

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