

Investigating Alloying Effect on Dislocation Mechanisms with *In Situ* and Multi-dimensional Characterizations

Qian Yu

Zhejiang University, Hangzhou, Zhejiang, China (People's Republic)

Mechanical properties of materials are highly related to dislocations structure and how they move in lattice. Alloying elements can significantly influence mechanical properties by tuning dislocation structure or behaviors. Solid solution strengthening mechanisms describes how the elastic interaction of dislocation and solute contributes to strength. However, alloying elements can make even stronger impact on mechanical properties beyond the random solid solution concepts. For example, alloying elements can strongly modify the dislocation core structure, resulting in abnormal increase of activation energy for dislocation motion; and the variations of local arrangement of alloying elements in concentrated solutions can also strongly tune dislocation behaviors through generating abnormal fluctuations of lattice friction. The broad field of electron microscopy (EM) instrumentation development holds great promise for addressing these problems due to its abilities to reach inherently high spatial resolution, to apply precise external fields, to visualize the behaviors of defects and to perform accurate measurements of the corresponding responses simultaneously. We applied multi-scale structure characterization, including high angle annular dark field scanning transmission EM (HAADF-STEM) and 3-dimensional dislocation tomography, and quantitative *in situ* TEM mechanical testing to investigate the correlations between the structural features such as atoms arrangement, dislocations and the mechanical properties in advanced alloys including Ti alloys¹, Ni-based super alloy², steels³ and high entropy alloys⁴⁻⁶. In this talk, we specifically focus on two subjects: 1) the intrinsic oxygen strengthening effect in titanium and 2) the dislocation mechanisms in high entropy alloys. By collaborating with theorists, we provide direct information as to the pathway by which the microstructure evolves and how the materials response to those dislocation activities, providing valuable information for the study of mechanical properties of advanced metals.

Given that solute atoms interact weakly with the elastic fields of screw dislocations, it has long been accepted that solution hardening is only marginally effective in materials with mobile screw dislocations. By using transmission electron microscopy and nanomechanical characterization, we found that the intense hardening effect of dilute oxygen solutes in α -Ti is due to the interaction between oxygen and the screw dislocations. First-principles calculations reveal that distortion of the interstitial sites at the screw dislocation core creates a very strong but short-range repulsion for oxygen that is consistent with experimental observations¹. Based on this, It was further found that Re atoms segregate at the tensile stress regions near the interfacial dislocation cores, forming the “Cottrell atmosphere”. The segregation process is facilitated by dislocation pipe diffusion, but can be regulated by thermal treatment. *In situ* TEM and scanning electron microscopy (SEM) straining studies reveal that the Re-decorated dislocation networks along the phase boundaries act as mechanical walls that effectively block dislocation motion and crack propagation. Theoretical analysis demonstrates that this remarkable alloying effect originated mainly from the interactions between the local composition strain of Re and the dislocation strains, leading to significantly stabilized interfacial dislocation networks².

We also found that significant concentration waves of elements exist in HEAs, particularly with the addition of Pd, which has very different atomic size and electronegativity comparing with other four elements. Consequently, the fluctuation of lattice friction became much stronger and dislocation behaviors

changed from planar slip to massive cross-slips⁴. Even in CrMnFeCoNi, the amplitude of the concentration wave can be ~10%. This feature, as a unique one in HEAs, differs this sort of alloys from the traditional alloys containing only one primary element. The key lock feature is that such concentration wave modulation occurs at a scale that is finer than precipitation hardening and is larger than that of traditional solid solution strengthening. It not only provides understanding for the intrinsic character of HEAs but also could enable researchers to custom design alloys in the future, exploring even superior materials properties.

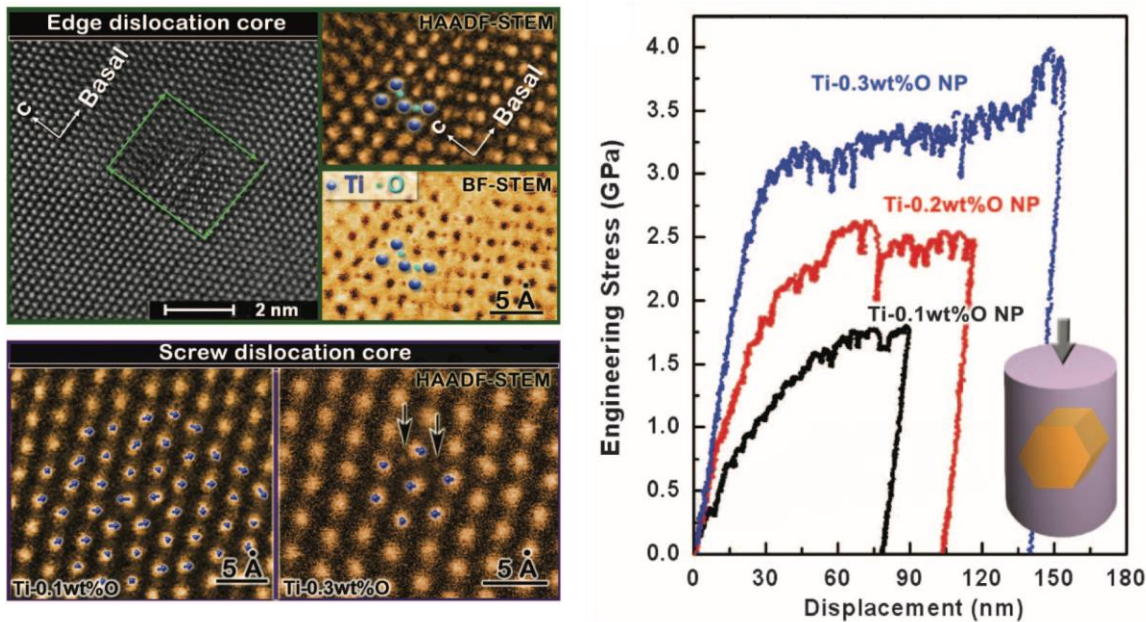


Figure 1. The HAADF STEM images of the edge and screw dislocation core with oxygen atoms segregation and its influence on mechanical properties of alloys.

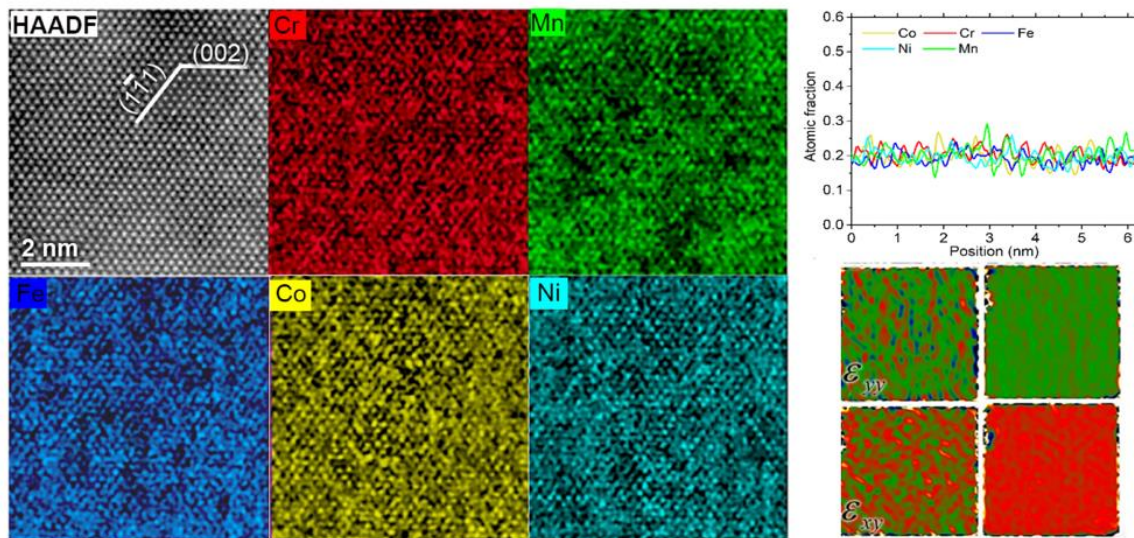


Figure 2. The atomic resolution EDS mapping of alloying elements in CrMnFeCoNi high entropy alloys and its corresponding strain mapping comparing with CrFeCoNiPd high entropy alloys.

References

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