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# Researchers find plastic deformation develops differently in titanium and zirconium

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Despite the many similarities between titanium and zirconium, researchers at CEA, CNRS and Université Claude Bernard Lyon 1 have demonstrated that plastic deformation develops differently in these two metals. It is commonly accepted that Ti and Zr should exhibit a similar response to mechanical stress. However, by combining microscopic experimentation and modeling techniques with GENCI and PRACE computing resources , the researchers have identified two different dislocation motions in these materials. Their goal is now to investigate and predict the mechanical properties of various innovative alloys. The results are published in the August 2015 issue of *Nature Materials*.

Titanium and zirconium, two crystalline metals used in industrial applications (particularly nuclear and aeronautical applications), have very similar electronic structures (same number of electrons in the outer shell). They also crystallize in a similar manner, i.e. when the atoms assemble into a crystalline structure, they adopt a similar geometry.

Despite the many similarities between these two metals, the researchers have unexpectedly shown that they respond differently to mechanical stress. By stretching a pure sample of each metal under a transmission electron microscope at various temperatures ranging from -170°C to +20°C, they have managed to observe and compare apparent line defects, i.e. dislocations evolving as a function of mechanical stress. Two types of dislocation behavior have been observed: dislocations passing jerkily through different planes (in the case of titanium), and dislocations slipping continuously on a single plane (in the case of zirconium).

## Simulation in support of experimental observations

In order to understand this difference in dislocation mobility, the researchers have modeled the dislocation core at the atomic scale using GENCI's Curie supercomputer. These simulations show that the dislocations may adopt two different configurations: one slipping easily and continuously, the other with difficulty. Each of these two configurations exists in both metals, but with a different degree of stability (or recurrence): the most stable dislocations observed in titanium are of the easily slipping type, as opposed to zirconium.

With this new understanding of plasticity in pure titanium and zirconium, it is now possible to model the plastic deformation behavior of corresponding alloys based on robust physical principles. Regardless of whether titanium or zirconium alloys are considered, the alloying elements used (particularly oxygen) have a significant effect on the material's plastic deformation behavior. The next step is therefore to investigate how the alloying elements interact with the different dislocation configurations and modify both their stability and mobility. There are important technological stakes involved, since zirconium and titanium alloys are structural materials commonly used in the nuclear and transport industries.

**More information:** "Dislocation locking versus easy glide in titanium and zirconium." *Nature Materials* 14, 931–936 (2015) DOI: 10.1038/nmat4340

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