

METALLURGY

Starting and stopping dislocations

A comparison of dislocation dynamics in two hexagonal close-packed metals has revealed that dislocation movement can vary substantially in materials with the same crystal structure, associated with how the dislocations relax when stationary.

Andrew M. Minor

Understanding what controls the movement of crystalline defects is key to designing higher performing structural alloys. Dislocation dynamics are complex, however, as exemplified by the behaviour of similar types of dislocation in near-identical crystal structures that can vary from one material to the next. This is the situation with dislocations in Ti and Zr, two hexagonal close-packed metals with similar properties and dislocation characteristics. Writing in *Nature Materials*, Emmanuel Clouet and colleagues¹ compare the motion of similar dislocation types in Ti and Zr, finding that their differing mechanical behaviour is related to the subtlety of the atomic configuration of the dislocations when they are stationary.

The mobility of individual defects controls the mechanical properties of structural materials. The more freely these defects can move, the more ductile the material is, which is important for both formability and for resisting the propagation of cracks. An individual dislocation can be most simply characterized by three crystallographic components: the plane they move on (glide plane), their direction on this plane (line direction) and the Burgers vector, which describes the displacement needed to form a closed circuit around the dislocation (essentially the size of the imperfection in the crystal). Knowledge of these three characteristics can reveal how a dislocation might move, and typically most materials have only a few classes of low-energy defects that exist and participate in deformation. The above characteristics can be determined experimentally, while modern computational tools allow the energetics of dislocation structures to be accurately calculated².

However, the study by Clouet and colleagues demonstrates that there is more to the story than simply the Burgers vector, glide plane and line direction of a dislocation. Atoms reconcile crystal imperfections locally by atomic rearrangements at the core of the defect, and

this core structure can resemble a complex arrangement of local faults and atomic displacements with different energetics for each configuration. Within the dislocation core, strains lie beyond simple elasticity theory and the atomic configurations can have multiple metastable states³. Previous studies have shown how dislocation core structures can strongly influence mechanical behaviour, for example in the case of body-centred cubic metals⁴, Ti (ref. 5) and Ti-based intermetallics⁶.

Clouet and co-workers revisit previous experimental observations⁷, in combination

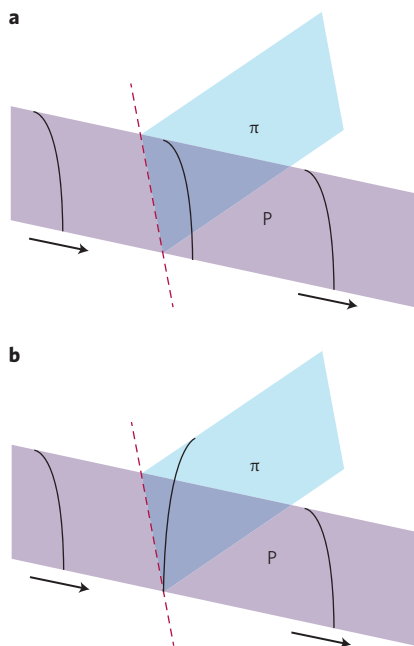


Figure 1 | Schematic of dislocation motion in Zr and Ti. **a**, In Zr, the dislocations moving on the prismatic (P) plane do not relax onto the pyramidal (π) plane, and hence propagate smoothly without interacting with the π plane (red line represents plane intersection). **b**, In contrast, when dislocations in Ti stop they transfer briefly onto the π plane. They only propagate on the P plane however, leading to their start-stop motion. Black arrows indicate direction of dislocation propagation.

with the current work, to compare the motion of similar dislocation types in Ti and Zr that should show little difference due to similar crystal structures. Instead, they find that dislocations in Zr move smoothly, essentially not stopping once they start, while in Ti they tend to stop and start, which is often described by 'jerky motion' or 'dislocation locking'. The difference in their movement is similar to comparing a car that is parked in a garage to one that is parked on the street; it is easy for the car parked on the street to set off because it is already on the street. This is the case for Zr, where the dislocation core lies on the same plane that it moves on. For Ti however, the dislocation core prefers to lie on a different plane to that on which it moves (Fig. 1), analogous to a car that has to park off the street every time it briefly stops. The result is impeded motion, similar to when dislocations split into smaller segments (partial dislocations), and in order for the dislocation to cross-slip onto new planes the disassociated segments need to first come together. This extra step leads to stopping and starting of the dislocation, which requires thermal activation.

The core structures of dislocations matter for dynamics. While it is possible for two materials to have dislocations with similar strain fields under similar applied stress conditions, whether those dislocations will move or not depends on their core structures. What is exciting about being able to predict the core structure of a dislocation through simulations is the idea that we can then computationally search for ways to change their motion, guided by insights into bonding, via detailed electronic structure calculations. Modern *ab initio* calculations of local density of states, as demonstrated by Clouet and colleagues¹, provide insight into why a certain core configuration might be stable or not. To change this, an obvious approach is to alter the electronic properties of the structure locally through solute additions⁸, similar to how semiconductors can be doped to change their properties.

The current study¹ shows how important dislocation core structures are to their motion, and points to strategies to engineer alloy mechanical properties by changing defect mobility. The result could be designer alloys with higher strengths, greater ductility and better performance in extreme environments. Metallurgists have long sought to understand the complex variations in mechanical behaviour that often arise from subtle changes in material chemistry. The work by Clouet *et al.* demonstrates

how integration of modern experimental and computational tools are now providing the link between composition and defect behaviour at the atomic level. □

Andrew M. Minor is in the Department of Materials Science and Engineering at the University of California, Berkeley, California 94720, USA, and the National Center for Electron Microscopy, Molecular Foundry, Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA. e-mail: aminor@berkeley.edu

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