Repulsive coupled screw dislocation pairs cause work hardening in bcc metals

The usability of metallic components depends on their resilience and work hardening during intentional or unintentional deformation. Dislocations collectively move and multiply when a metal is strained, which leads to increased dislocation density and thereby work hardening and increased flow stress upon straining. Face-centered cubic (fcc) metals such as aluminum typically show stronger strain hardening than body-centered cubic (bcc) metals such as tungsten. Current work hardening models assume flow stress is inversely proportional to average dislocation spacing due to the dislocation density dependence. These models work at higher temperatures especially for bcc metals. Tungsten, however, extensively work hardens at room temperature. This has been attributed to the behavior of screw dislocations at lower temperatures in tungsten.

Using discrete dislocation dynamics simulations, researchers at Karlsruhe

Institute of Technology (KIT), Germany, including Daniel Weygand, have now found that in bcc metals such as tungsten, coupled repulsive screw dislocations push one another on unexpected slip systems, influencing the hardening behavior of the material. This is a new mechanism not reported previously. Their colleagues at CEMES-CNRS, France, confirmed this mechanism experimentally in tungsten.

As reported in a recent issue of *Nature Communications* (<https://doi.org/10.1038/s41467-020-18774-1>), the research team at KIT showed that specific repulsive dislocation pairs couple together depending on the external load condition. In simulations, the researchers placed one screw dislocation along glide system $(\bar{1}01)[111]$ (dislocation I) and another screw dislocation along glide system $(011)[11\bar{1}]$ (dislocation II). Tensile loading was applied to the crystal along the $[\bar{1}49]$ direction. The dislocations were initially ~ 50 nm apart. With a resolved shear stress of ~ 1.8 GPa, dislocation I begins to glide. It reaches a velocity of ~ 1.05 nm/s while dislocation II is initially immobile. As dislocation I closes the distance to about 9.5 nm, it causes dislocation II to glide. “From that point on, the velocity of dislocation II increases rapidly to match the velocity of dislocation I,” the research group writes, to the point where they glide collectively.

“The most important observation is that pairs of screw dislocations, which are elastically repulsing each other, show a coupled gliding,” says Vaclav Vitek, Professor of Engineering and Applied Science Emeritus at the University of Pennsylvania who was not involved in this study. “The coupling of the two dislocations enhances the plastic strain without requiring an additional applied stress and thus

the strain-hardening rate is effectively lowered.”

In situ transmission electron microscopy confirmed these results when examining repulsively oriented screw dislocations in strained thin films of a tungsten single crystal. At a temperature of 300 K, the distance between the dislocations was ~ 24 nm when coupled motion occurred. As both dislocations move at the same speed, they do not cross each other; in other words, there is no cross slip.

“During coupled motion the second dislocation (slip system 2) contributes to the total plastic shear rate on slip system 2, due to dislocation glide on slip system 1, even though macroscopically the resolved shear stress is below its [critical resolved shear-stress],” the researchers write. The results, the research team reports, may lead to a better understanding of the increase in ductility of highly deformed bcc metals.

The coupling mechanism of screw dislocations is important to explain the observed extended work hardening regime for tungsten single crystals at room temperature (and lower temperatures). The repulsively oriented screw dislocations glide collectively without an applied stress, rather than obstruct motion, as understood conventionally. The results also challenge current notions of internal stresses in bcc metals and how these affect dislocation movement. This may explain the enhanced ductility observed in heavily cold-rolled tungsten, with high dislocation densities with increased density of screw dislocation pairs that may trigger such coupled motion.

Vitek says, “For applications it implies that the flow criteria used in continuum analyses of deformation of complex structures made from bcc metals need to be modified such as to take into account the coupling of dislocations that move for a given loading with those that, in the usual considerations of the effect of applied loading, would not move.”

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In situ transmission electron microscopy difference image showing motion of a pair of screw dislocations in single crystal tungsten. In body-centered cubic metals such as tungsten, screw dislocations are pushed ahead of one another, showing coupled gliding leading to major deformation. Graphic: D. Weygand, KIT, D. Caillard, CEMES.