Dislocation does the twist with a double helix

There have been moments of triumph in the history of crystal dislocations. Sir Charles Frank showed in 1949 that a screw dislocation provides surface steps for crystal growth. Without the screw dislocation, crystal growth from the vapor phase would require unrealistically large supersaturations. John D. Eshelby showed in 1953 that a coaxial screw dislocation in a finite cylinder can introduce opposing shear stresses at the end surfaces, which produce what came to be known as the Eshelby twist. The Eshelby twist is directly proportional to the magnitude of the Burgers vector of the screw dislocation, **b**, and inversely proportional to the square of the cylinder radius, R. With the availability of nanomaterials, the Eshelby twist is becoming prominent.

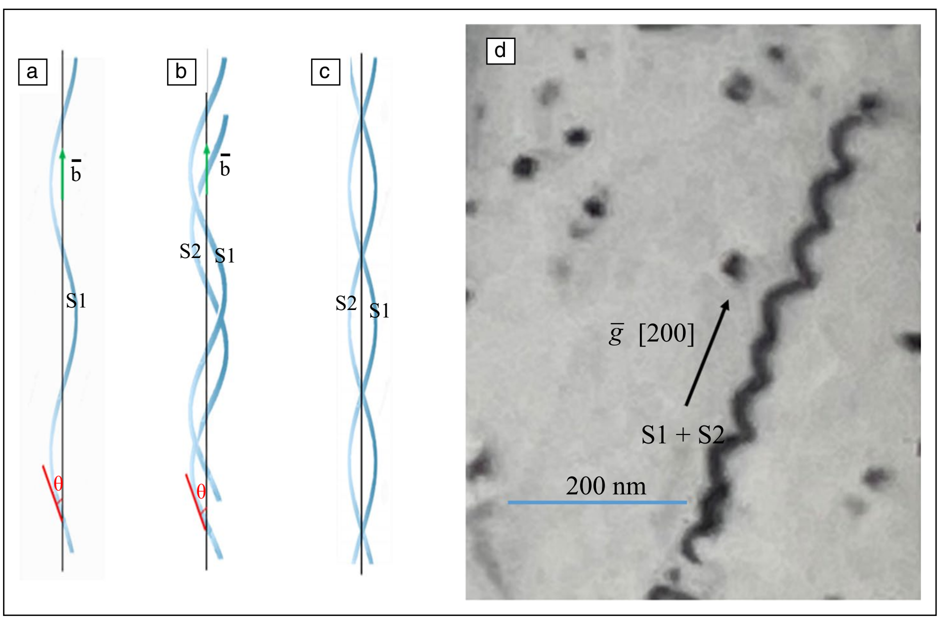
The next advance took place when S. Amelinckx et al. showed in 1957 that a screw dislocation can become helical by absorbing vacancies. Then a problem arose: the magnitudes of Burgers vectors experimentally measured for crystalline structures with hollow cores and Eshelby twists were found to be considerably larger than the Burgers vectors of elementary screw dislocations in a number of materials including germanium sulfide (GeS), lead sulfide (PbS), lead selenide (PbSe), and magnesium oxide (MgO). To solve this puzzle, J. Narayan, who is the John Fan Family Distinguished Chair Professor at North Carolina State University, proposed in a published perspective that the helical dislocations having some edge and mostly screw character can pair up through attractive interaction to form a ***double*** helix (*Materials Research Letters*, https://doi.org/10.1080/21663831.2021.1973131).

This attractive interaction between two helices is derived through the edge component of mixed dislocations and from the presence of vacancy jogs (pure screw dislocations with no edge component repel each other and cannot form a helix). Narayan proposes a "rule of mixture" for the effective Burgers vector **be**:

$$\mathbf{be} = 2\delta\mathbf{b}\cos\theta + (1 - \delta)\mathbf{b}\cos\theta,$$

where θ is the angle of the helix and δ is the fraction of the double helices. The accompanying figure shows single helices that combine to form double helices. It is interesting to note the similarities between a single helical screw dislocation (**Figure a**) and single strand ribonucleic acid (RNA), and double helix dislocations (**Figure c**) and deoxyribonucleic acid (DNA) structures with two strands. Narayan's proposal can be explained with numerical examples. In GeS, the Burgers vector (**b**) calculation based on the Eshelby twist gives a value of 1.04 nm compared to the experimentally measured value of 1.75 nm. If the material had 71% double helices (and 29% single helices), the previous equation with a helix angle of 10 degrees correctly predicts the observed value. Similarly, 45% double helices would explain the measured value in PbS.

In a follow-on article (*ACS Omega*, https://doi.org/10.1021/acsomega.2c03501) J. Narayan and R.J. Narayan presented direct evidence for the formation of a double helix in MgO (see figure). In their experiments, thermal annealing of MgO supplied vacancies to facilitate the formation of single helices, some of which combined to form double helices. The percentage of double helices in this study is estimated as 30 percent. Narayan says, "Single and double helices combined with other features can produce very large Burgers vectors and Eshelby twists. These concepts can unravel the mechanism for the formation of nanopipes and micropipes with hollow cores and nanotubes." The



Helical screw dislocation in MgO. (a) A single helical screw dislocation ($n = 1$) at S1 with a constant helix angle θ along the entire length of the dislocation; (b) formation of a double-helix dislocation with another dislocation S2, which is shifted by a quarter of a pitch (λ/4) along the axis; (c) shift is half (λ/2) of a pitch; and (d) transmission electron micrograph of a double helix with two screw dislocations of a/2 [101] Burgers vector. There is an attractive interaction between the two (mixed) dislocations through the edge component and vacancy jogs, similar to hydrogen bonding between two DNA strands. Credits: J. Narayan and R.J. Narayan; *ACS Omega*.

helical dislocations can have unique electrical, optical, magnetic, and superconducting properties, leading to novel nanoscale solid-state devices.

Yuntian Zhu, Chair Professor at the City University of Hong Kong, who is an internationally known expert in this area (and not involved in the present work) says, “The discovery of double helix of screw dislocations by Prof. Narayan has revolutionized our understanding of crystal growth from nanoscale to mesoscale. It provides an explanation on the formation of hollow-core nanopipes and large Eshelby twists. The formation of double helix of screw dislocations is a natural consequence of dislocation climb in the presence of vacancy defects, the research pioneered by Narayan and Washburn over a half century ago (J. Narayan, J. Washburn, *Philos. Mag.* **26**, 1179 [1972]).”

N. Balasubramanian