Discovery of Double Helix and Impact on Nanoscale to Mesoscale Crystalline Structures
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ABSTRACT: Screw dislocations play a significant role in the growth of crystalline structures by providing a continuous source of surface steps which represent available sites for crystal growth. Here, we show that pure screw dislocations can become helical from the absorption of defects (e.g., vacancies) and develop an attractive interaction with another helical dislocation to form a double helix of screw dislocations. These single and double helices of screw dislocations can result in the formation of interesting nanostructures with large Eshelby twists. We have previously proposed the formation of a double helix of screw dislocations to explain large Eshelby twists in crystalline nanostructures (Mater. Res. Lett. 2021, 9, 453–457). We now show direct evidence for the formation of a double helix during thermal annealing of screw dislocations. The large Burgers vectors associated with these dislocations are used to explain the presence of large Eshelby twists in PbSe and PbS (NaCl cubic structure) and InP and GeS (wurtzite hexagonal structure) nanowires. These single- and double-helix screw dislocations can also combine to create even larger super Burgers vectors. These large effective Burgers also unravel the mechanism for the formation of nanotubes and micropipes with hollow cores and nanotubes with Eshelby twists in technologically important materials such as SiC, GaN, and ZnO that are utilized in a variety of advanced solid-state devices.

1. INTRODUCTION
Screw dislocations with Burgers vectors parallel to dislocation lines play a critical role in crystal growth across the scale ranging from nanostructures to large crystalline structures as well as in determining the mechanical properties of solid-state materials.\(^1\)\(^-\)\(^8\) The creation of a screw dislocation can be visualized by partially slicing into a crystal along a specified plane and then displacing one face with respect to the other by a lattice (Burgers) vector. The boundary of this cut represents a screw dislocation along which lattice planes are arranged in a helical way.\(^9\) This helical structure can provide a continuous source of surface steps for crystal growth along the axes of screw dislocations. This concept, originally proposed by Sir Charles Frank, solved a longstanding challenge in materials science and explained crystal growth at supersaturations as low as 1%.\(^10\) Without these dislocations, crystal growth from the vapor phase requires supersaturations exceeding 1.5. The crystal growth velocity is directly proportional to the fraction of sites available for attachment during crystal growth, which can be provided by the steps associated with emerging screw dislocations. This self-seeding crystal growth mechanism is applicable across the scale ranging from nanowires to whiskers.\(^5\)\(^-\)\(^8\) Moreover, it can overcome the utilization of catalysts for the growth of nanostructures (e.g., nanowires) and thus minimize impurity contamination. Catalysts are associated with contamination by undesirable impurities; a few contaminant atoms can lead to large local concentrations and changes in properties.\(^2\)\(^-\)\(^5\)

However, dislocations are nonequilibrium defects; their presence raises the system energy, which is proportional approximately to the square of the magnitude of the Burgers vector. With an increasing magnitude of the Burgers vector of the dislocation, the system can lower its energy by creating a free surface along the core of the dislocation (a hollow core) and stay in a local equilibrium. Frank proposed the formation of hollow cores of screw dislocations for crystal structures with large Burgers vectors.\(^7\) He derived the size of the hollow core by equating the incremental change in strain-energy density by using linear elasticity theory to the change in the surface energy of the hollow core. However, the size of the Burgers vectors obtained was too small to account for experimental observations.\(^2\)\(^-\)\(^5\) By taking into account nonlinear effects empirically, Frank obtained higher values of the Burgers vectors needed to stabilize the formation of hollow cores.\(^7\) However, these estimates still do not correctly take into account the true core energy contributions, which can be handled only by atomistic calculations and not by continuum linear elasticity theory.\(^11\)\(^,\)\(^12\)
Experimentally observed values for the Burgers vectors, however, are considerably higher than these estimates and elementary Burgers vectors derived from crystal structures.\textsuperscript{13,14} This is particularly relevant to hexagonal crystal growth along the c-axis having the largest Burgers vector. Dudley et al.\textsuperscript{15} found that elementary dislocations in 6H-SiC ($c = 1.51$ nm) were not hollow, and the smallest hollow core dislocation had a Burgers vector of two unit cells (3.0 nm). The Burgers vector in the micropipe was found to have a height of at least four to 12 unit cells (18 nm) to stabilize a hollow core dislocation.\textsuperscript{14,16} More recent work on the growth of ZnO nanotubes likewise demonstrated the role of screw dislocations, but the measured effective Burgers vectors were three to four times higher than the magnitude of c-vectors.\textsuperscript{17}

There is another interesting consequence associated with the presence of screw dislocations during crystal growth. Crystal growth is associated with a coaxial screw dislocation inside a finite cylinder; the end surfaces are associated with counteractive shear stresses that generate the Eshelby twist (a torque and a twist).\textsuperscript{1,4,5} Since the Eshelby twist is directly proportional to the magnitude of the Burgers vector of the screw dislocation and inversely proportional to the square of the cylinder radius, it does not play a major role in large size crystals. In contrast, in screw-dislocation aided nanostructure growth (e.g., nanowires), Eshelby twist can provide helically twisted nanostructures with applications in nanoelectronics, nanophotonics, and energy harvesting.\textsuperscript{2–3} Again the same difficulty arose in the interpretation of Eshelby twists. The magnitudes of Burgers vectors experimentally measured for Eshelby twists were considerably larger than the Burgers vectors of elementary screw dislocations.

Associated with the discovery of the double helix, we have solved this longstanding puzzle in the field of dislocations and their role in crystal growth and related phenomena such as Eshelby twist.\textsuperscript{1} We showed the transformation of pure screw dislocations into helical dislocations and the formation of a double helix of screw dislocations via the pairing of two helical dislocations (similar to the DNA structure). Here, we describe evidence of the formation of a double helix of screw dislocations in MgO having NaCl structure after thermal annealing, which supplied vacancies. The creation of a double helix may start with a single helical dislocation at the initial stages, where another single dislocation can join subsequently through attractive interaction. Now we can explain the large effective super Burgers vectors needed to rationalize the formation of nanotubes, nanotubes, and micropipes, including the large Burgers vectors found in Eshelby twist. We derive the strategy for reducing the formation of nanotubes and micropipes and discuss the role of single and double helix screw dislocations with Eshelby twists in creating novel nanostructured materials with improved properties.

2. RESULTS AND DISCUSSION

2.1. Role of Screw Dislocations. The role of screw dislocations in crystal growth is well established, where they provide a continuous source of available growth sites. Since self-energy of a screw dislocations increases as the square of the Burgers vector in the elastic region, Frank predicted the formation of hollow cores for dislocations with large Burgers vectors, such as screw dislocations along the c-axis in hexagonal crystals of 6H-SiC.\textsuperscript{7} These dislocations can lead to the formation of nanotubes and micropipes in hexagonal crystal structures of SiC, GaN, and AlN, which are highly undesirable, known as “killer defects” for light-emitting diodes, high-power, and high-frequency devices.\textsuperscript{14} By unraveling the mechanism of formation, we should be able to reduce the number density of nanotubes and micropipes and alleviate their harmful effects. The screw dislocations with hollow cores can also lead to the formation of nanotubes as observed in the case of ZnO.\textsuperscript{17}

Frank proposed the formation of hollow cores of screw dislocations for crystal structures with large Burgers vectors.\textsuperscript{7} He considered the change in strain energy density and surface energy of a cylinder along the dislocation in the elastic region. The change in energy, $\Delta E$, equals gain in surface energy minus the corresponding loss in the strain energy

$$\Delta E = 2\pi \gamma dr - (1/2\mu r^2) 2\pi dr$$  \hspace{1cm} \text{(1)}$$

where $\mu$ is the shear modulus, $\gamma$ is the surface energy of the hollow tube, $b$ is the magnitude of the Burgers vector, and strain $\varepsilon = b/2\pi r$ at the surface of the cylinder of radius $r$. From $d\varepsilon/dr = 0$, he derived the radius of the hollow core ($r$) as

$$r = \frac{b^2}{8\pi^2 \gamma}$$  \hspace{1cm} \text{(2)}$$

By taking into account nonlinear effects empirically, Frank estimated higher magnitudes of Burgers vector in the range of $20\pi \gamma / \mu$ to $66\pi \gamma / \mu$ for the formation of hollow cores. However, this model involved an unrealistic assumption that for strains greater than 0.1, as those involved in the dislocation core, the strain energy is constant (at $\mu/200$).\textsuperscript{7}

An alternative approach to obtain the hollow core radius is based upon minimization of total energy ($E_T$) of the system, including the core energy of the dislocation, where

$$E_T = 2\pi \gamma + E_c + \mu b^2 / 4\pi (\ln R/r)$$  \hspace{1cm} \text{(3)}$$

where $\gamma$ is the surface of the hollow core, $E_c$ is the core energy, and the third term is the energy of the dislocation in the linear elastic region. By minimizing ($dE_c/dr = 0$), we obtain the core radius as

$$r = \frac{\mu b^2}{[4\pi (2\pi \gamma - \alpha)]}$$  \hspace{1cm} \text{(4)}$$

where $dE_c/dr = -\alpha$. If we take $E_c$ to be constant, we obtain the same result as eq 2. However, $E_c$ needs to be handled by atomistic calculations, as the core energy distortions are nonlinear. From detailed atomistic calculations, the nonlinear dislocation core energy contributions in Si, Ge, and diamond were noted to be a strong function of $r$, $b$, and dislocation sense vector.\textsuperscript{11,12} The negative value of $\alpha$ signifies that core distortions decrease with increasing $r$. Similar calculations are needed for other structures, such as SiC, GaN, and ZnO, to estimate $\alpha$.

At present, these estimates and experimentally observed values for the Burgers vectors are considerably higher than elementary Burgers vectors derived from the crystal structures. The observation of hollow cores and micropipes in (0001) oriented 6H-SiC ($a = 0.307$ nm, $c = 1.51$ nm), GaN ($a = 0.319$ nm, $c = 0.519$ nm), and ZnO ($a = 0.325$ nm, $c = 0.520$ nm) qualitatively support the concepts proposed by Frank. However, the magnitude of the Burgers vectors associated with nanotubes and micropipes was found to be significantly larger than the respective c-vectors. As discussed in ref 15, elementary dislocations in 6H-SiC were not hollow, and the smallest hollow core dislocation had a Burgers vector of two unit cells (3 nm). Others\textsuperscript{13,16} reported that the Burgers vector in the micropipe needs to have a height of at least four to 12 unit cells (18 nm) to stabilize a hollow core dislocation. More recent work on the growth of ZnO nanotubes confirmed the role of screw
dislocations where the effective Burgers vector was measured to be three to four times the magnitude of the c-vectors.

### 2.2. Formation of Single Helix and Double Helix Screw Dislocations

#### 2.2.1. Formation of Helical Screw Dislocations

In the following sections, we show that larger effective or super Burgers vectors are possible by the formation of helical screw dislocations, which can pair up to form a double helix and attract additional helical screw dislocations. A pure screw dislocation can attain helicity via dislocation self-climb by absorbing point defects throughout the growth process or thermal annealing, as shown in Figure 1a. It is found that the interactions between the hydrostatic stresses of vacancies and the shear stresses of screw dislocations are very weak. It should be noted that local jogs as well as thermal stress fluctuations can introduce local edge components, which are able to interact with the hydrostatic stresses of vacancies. There is an attractive interaction energy between two jogs (\(E_i\)): it is given by

\[
E_i = \mu b^2 a^2 / [8\pi L(1 - \nu)]
\]

where \(b\) is the Burgers vector magnitude, \(\mu\) is the shear modulus, \(L\) is the spacing between the jogs, \(a\) is the length of the jog, and \(\nu\) is Poisson’s ratio. As the absorption of vacancies continues, the edge component of the screw dislocations increases, and the vacancy interactions grow stronger. This causes helix angle \(\theta\) (as shown in Figure 1a) to stay constant along the entire length of the dislocation; it is related to the radius \(r_h\) and pitch \(\lambda\) of the helix as \(\theta = \tan^{-1}(2\pi r_h/\lambda)\).

The equilibrium condition as a result of absorption of vacancies is achieved when the change in energy per unit length of the helix with \(r_h\) equals the change in energy of vacancies which can be expressed as

\[
d(\Delta E_h) / dr_h = d(N\Delta G_i) / dr_h
\]

where \(\Delta G_i\) is the formation energy of a vacancy, which is equal to \(kT\ln(c/c_0)\).

This results in a relationship between supersaturation of vacancies \(c/c_0\), radius, and pitch for the formation of a helix, which is given by

\[
kT \ln(c/c_0) = 2\pi \Omega \lambda / [b(2\pi r_h)^2 + \lambda^2 \rho^2]
\]

Here we assume that the sample is quenched from a higher concentration \(c\) to lower \(c_0\).

It is seen from eq 10 that \((2\pi r_h)^2 + \lambda^2\) is a constant for a particular supersaturation of vacancies; this equation implies that as \(r_h\) decreases, then \(\lambda\) must increase. For very small \(r_h\), which is expected for the growth of nanostructures, the critical pitch length \(\lambda^*\) is provided by

\[
\lambda^* = 2\pi \Omega \rho (bkT \ln(c/c_0))^{-1}
\]
Figure 2. Formation of stacks of loops from helical screw dislocations due to vacancy diffusion as well as punching into a stack of vacancy loops in (001) MgO after high-temperature annealing at 1273 K: (a) TEM micrograph taken with diffraction vector [200] showing a/2[110] loops at S3 and a/2[110] loops at S4 and (b) TEM micrograph of the same sample in a different region taken with diffraction vector [200], showing a/2[110] loops at S4 and a/2[1–10] loops at S5.

If the pitch $\lambda > \lambda^*$, the helix free energy declines with increasing $r_0$; the helix grows through absorbing vacancies and turns eventually into a stack of vacancy loops, as shown experimentally below in Figure 2. However, if $\lambda < \lambda^*$ then the diffusion of vacancies via thermal activation is needed to attain the critical value of $\lambda^*$. Once a helix begins to form, it is unstable with regard to radial growth. For $\Omega \sim b^3/4$ for GeS (orthorhombic) and $b^3$ for PbS (cubic), $\tau = 20$ eV/nm estimated from refs 11 and 12, supersaturation $c/c_0 = 10$, $kT = 56$ meV [2], then ($\lambda^*$) is estimated to be 100 nm for GeS, and 120 nm for PbS with $kT = 73$ meV. The helix radii are estimated to be over the range from 1 to 3 nm for helix angles that vary from 5 to 10$^\circ$.

2.2.2. Formation of Double Helix of Screw Dislocations. The pairing of two pure screw dislocations to account for the experimentally observed larger Burgers vectors has been problematic since two parallel pure screw dislocations exhibit repulsive interactions. The repulsive force ($F$) is given by $F = \mu b^2 \cos 2\phi [2\pi r(1 - \nu)]$, where $r_0$ is separation between the two dislocations. However, a pure screw dislocation can acquire jogs through the absorption of vacancies, which are present during the growth process. The vacancy absorption imparts an edge component, and the screw component adds helical character. The jogs generated via absorption of vacancies in a helical dislocation interact with those in other helical dislocations. The attractive interaction is the basis for the pairing of two helical dislocations and the formation of a double helix of screw dislocations. Moreover, there is an attractive interaction between two helical dislocations derived via edge components that were obtained via vacancy absorption. This attractive interaction force ($F_A$) per unit length for two parallel edge dislocations may be estimated using

$$F_A = \mu b^2 \sin^2 \theta \cos \Phi \cos 2\phi [2\pi(1 - \nu)]$$

where $\theta$ is the helix angle, $b \sin \theta$ is the edge component, $\Phi$ is the angle between dislocation distance vector $r$ and dislocation plane, and $F_A$ is attractive (negative) for $\Phi$ in the range of 0–45$^\circ$ and repulsive beyond that.

With the above attractive interactions, we envisage that two helical screw dislocations can pair up to form a double helix of screw dislocations with a larger effective Burgers vector. Figure 1b depicts double helix formation where there is a relative shift of $\lambda/4$; for a shift by $\lambda/2$, the double helix is provided in Figure 1c. Two helical dislocations may alter their relative positions due to their origin and growth conditions. An additional attractive interaction may be derived from vacancy jogs present in the helical dislocations. It is important to note the similarities between single helical screw dislocation (Figure 1a) and single-stranded ribonucleic acid (RNA) molecules as well as between double-helix dislocations (Figure 1c) and double-stranded deoxyribonucleic acid (DNA) molecules.

The formation of a single helix as a result of vacancy absorption has been studied ever since the first report by Bontinck and Amelinckx. More recently, the formation of single helix dislocations was reported by Haley et al. in Fe-9Cr alloys, where screw dislocations acquired helical character by absorption of vacancies produced by neutron irradiation. Since the neutron damage produced vacancy and interstitial (Frenkel) pairs, the absorption of vacancies by screw dislocations enhanced the clustering of interstitials in the form of loops in the vicinity of helical dislocations. In this study, we describe the formation of the single and double helix screw dislocations in MgO as a function of annealing at high temperatures. Before annealing, these MgO crystals contained a high density of screw,
mixed, and edge dislocations associated with a deformation treatment in MgO. Upon thermal annealing at 1273 K, which introduced an ample supply of vacancies from the free surface, screw dislocations acquired helical character by absorbing vacancies. The helical dislocations then paired up and formed a double helix, as shown in Figure 1d. This micrograph was taken with diffraction vector \( g = [200] \), with [001] surface normal. The Burgers vector from \( g.b \) and \( g.bu \) contrast analysis was determined to be \( a/2[101] \) with sense vector \( u = [101] \). The observed width of the image is consistent with a double helix of screw dislocations. The contrast analysis was determined to be \( a/2[101] \) with sense vector \( u = [101] \). The observed width of the image is consistent with a double helix of screw dislocations.

The vacancys–dislocation interaction increases with the absorption of vacancies, which in turn increases the attractive edge component consequently. With continued absorption of vacancies, helical dislocations transform into a stack of vacancy loops with separation equal to the pitch and loop radius equal to the radius of the helix, as shown in Figure 2. From the contrast analysis, it is determined that the stacks of prismatic loops on (101) planes at S3 (Figure 2a) are the product of a single helix originally oriented along the [101] direction and (101) plane, which lies at 45° from the surface normal [001]. The stacks of loops at S4 (Figure 2a,b) are derived from an \( a/2[110] \) screw dislocation oriented along the [110] direction, whereas the stacks at S5 result from \( a/2[110] \) screw dislocation laying along the [110] direction. These \( a/2[110] \) and \( a/2[110] \) loops lie edge-on in the [001] sample orientation. It is important to note that the length of stacks at S4 and S5 is larger as these dislocations lie nearly parallel to the [001] specimen. From Figure 2 (S4 and S5), the helix pitch is estimated to be 50 nm and \( r_n = 5 \) nm, giving a helix angle of 30–35° and a vacancy supersaturation of \( (c/c_0) \) of 2.5 during annealing at 1273 K (assuming \( \Omega = b^2 r \) and \( r = 20 \text{ eV/nm} \)).

The smaller \( \lambda \) at S5 compared to S4 is consistent with the presence of a double helix and a single helix, respectively, as \([2\pi r / \lambda]^2 + \lambda^2] \) is constant for a specified supersaturation of vacancies.

The formation of nanopipes and micropipes requires the formation of dislocations with large Burgers vectors. We propose that this can occur by the formation of single helix and double helix of screw dislocations, which can start the nucleation process. Other helical dislocations can then join in through the surface interaction with the hollow core as proposed by Pirouz. From the above discussions about the formation mechanism, we can derive strategies for reducing the number density of nanopipes and micropipes. To reduce the formation of nanopipes and micropipes, we need to reduce the formation of dislocations with large super Burgers vectors. This will require the reduction of the helical dislocations, which can be accomplished by controlling the supply of vacancies via reducing growth temperature during the initial stages of growth. The reduced temperature will also lower the dislocation mobility, which will inhibit the formation of dislocations of larger Burgers vectors. In ZnO, the growth of nanotubes was found to be driven by axial screw dislocations, where self-perpetuating growth spirals enabled the formation of hollow tubes. However, the magnitude of Burgers vector estimated from surface height measurements was found to be 3–4 times higher than the magnitude of elementary Burgers vector \( (0.520 \text{ nm in ZnO}) \). These results can be rationalized by a combination of single helix and double helix of screw dislocations, which develop during the growth of nanotubes.

2.3. Impact of Double Helix on Eshelby Twist. In 1953, Eshelby noted that the axial screw dislocation generates a torque in a rod of finite length, which results in an elastic twist in crystalline structures. During growth of a crystal, a coaxial screw dislocation within a finite cylinder with end surfaces generates counteractive shear stresses, which generate an Eshelby twist (a torque and a twist). The Eshelby twist is inversely proportional to the square of the cylinder radius; it does not have a major role in large size crystals. In contrast, in screw dislocation aided nanostructure growth (e.g., nanowires), the Eshelby twist can result in interesting helically twisted nanostructures.

Again, the same difficulty arose in the interpretation of the Eshelby twist. The magnitudes of the Burgers vectors derived from experimentally measured Eshelby twists were considerably higher than the Burgers vectors of elementary screw dislocations.

Following the Eshelby twist model, the twist per unit length (\( \alpha \)) is given by

\[
\alpha = -\pi b (\pi R^2)^{α-1}
\]

where \( b \) is the magnitude of the Burgers vector of the screw dislocation and \( R \) is the radius of the nanowire cylinder. The negative sign signifies that the stress, which produces torque for the Eshelby twist, is opposite to that in the bulk, which is required to satisfy the boundary condition of stress zero at the free surface. The Eshelby’s formula is not valid at the ends of the cylinder. The length over which Eshelby twist completes its cycle is given by \( 2\pi/\alpha \). The \( n = 1 \) case corresponds to Eshelby’s original model with a single pure screw dislocation. At the time, the \( n = 2 \) case was ignored since the pairing of two parallel screw dislocations was deemed unstable due to a repulsive interaction.

In the case of screw dislocations with hollow cores and nanotubes, the Eshelby twist is reduced according to

\[
\alpha = -\pi b (\pi R^2 + \pi r^2)^{α-1}
\]

where \( R \) and \( r \) are the outer and inner radii of the hollow core structures and nanotubes.

With the introduction of helical dislocations, the Eshelby twist equation for a single helix should be modified to

\[
\alpha = -b \cos \theta (\pi R^2)^{α-1}
\]

where \( \theta \) is the angle of the helix.

For a double helix, the Eshelby twist equation should be modified to

\[
\alpha = -2b \cos \theta (\pi R^2)^{α-1}
\]

where \( \theta \) is the helix angle, which remains constant along the entire dislocation line.

From their work on PbSe nanowires with NaCl structure, Zhu et al. reported large Eshelby twists where the magnitude of the Burgers vector \( b \) was noted to be 1–3 times the Burgers vector \( (100) \) instead of the normal Burgers vector \( a/2[110] \). The generation of dislocations with the \( (100) \) Burgers vector was reported earlier in MgO having the NaCl structure.

Similarly, Bierman et al. described screw dislocation nanowire growth in PbS (a NaCl structure with \( a = 0.594 \text{ nm} \) and reported an...
effective Burgers vector \((0.6 \pm 0.2 \text{ nm})\) that was much higher than elementary Burgers vectors.\(^4\)

More recent work by Liu et al. involving growth of GeS (an orthorhombic structure with \(c = 1.04 \text{ nm}\)) nanowires indicated that axial screw dislocations created a discretized crystallographic twist that occurred along the \(c\)-axis.\(^5\) This resulted in helically twisted nanowire structures that were explained using Eshelby’s twist model.\(^16,19\) However, the effective Burgers vector \((b = 1.75 \text{ nm})\) was found to be far larger than the \(b = 1.04 \text{ nm}\) associated with [0001] dislocations, expected from the Eshelby’s model. In the following section, we note that the results from these experiments are rationalized by referring to growth via single and double screw dislocations with helical configurations. Since the screw component \((b \cos \theta)\) of the helical dislocation is involved with the growth process, the double helix effective Burgers vector that contributes to the growth process is \(2b \cos \theta\); this value is slightly smaller than \(2b\). When both single helix and double helix dislocations contribute to the growth process, we can write

\[
2\delta b \cos \theta + (1 - \delta) b \cos \theta = b e
\]

(17)

In this equation, \(\delta\) is the fraction of double helix, \(\theta\) is the angle of the helix, \((1 - \delta)\) is the fraction of single helix, and \(be\) is an experimentally observed average value for the Burgers vector. In the case of GeS growth,\(^1\) where \(b = 1.04 \text{ nm}\) and \(be = 1.75 \text{ nm}\), \(\delta\) was noted to be 71% and 69% with helix angle values of 10 and 5 degrees, respectively. For PbS\(^3\) with \(b = 0.42 \text{ nm}\) and \(be = 0.6 \text{ nm}\), \(\delta\) was calculated as 45% and 43% with helix angle values of 10 and 5\(^\circ\), respectively. To describe a higher level of double helices in GeS than in PbS, it should be noted that GeS exhibits orthorhombic (pseudo hexagonal) structure; the major dislocations involved in the growth process are \(c\)-dislocations. The screw dislocations are able to significantly reduce their energy by growing in (0001) directions.\(^11,12\) On the other hand, PbS exhibits a cubic NaCl structure (as in MgO) in which there are no dominating Burgers vectors for screw dislocations. As such, growth in PbS\(^5\) takes place along the (100) direction with mixed \(a/2\) (110) dislocations. In the case of PbS\(^5\) (NaCl or MgO structure), it is envisaged that the core of an \(a\) [100] dislocation splits into \(a/2\) [110] and \(a/2\) [1\(\overline{1}\)0] dislocations as demonstrated for MgO.\(^20\) Here, two \(a/2\) [110] and \(a/2\) [1\(\overline{1}\)0] Burgers vectors combine to provide an effective \(a\) [100] Burgers vector during crystal growth along the [100] direction. This is equivalent to \(\delta = 1\) and \(\theta = 45^\circ\) in eq 17; we obtain \(b_e = 0.594 \text{ nm}\), which is in good agreement with the experimental observations of 0.6 nm for PbS.

In summary, we have shown the impact that a single helix and double helix of screw dislocations can have on crystal growth and formation of nanostructures in solid-state materials. Screw dislocations can have critical roles in the growth of crystalline structures by providing a continuous source of surface steps, which represent available sites for crystal growth. However, experimentally derived Burgers vectors are found to be far larger than elementary Burgers vectors derived from the crystal structures. This longstanding puzzle has been solved with the discovery of stable double helices of screw dislocations. Two parallel straight screw dislocations exhibit a repulsive interaction and cannot pair up to increase the magnitude of the effective Burgers vector. However, attractive interactions can develop if these screw dislocations take on a helical character. We have shown that pure screw dislocations can become helical by the absorption of defects (e.g., vacancies) and develop attractive interactions with another helical dislocation to form a double helix of screw dislocations. The single helix and double helix of screw dislocations can also combine to create even larger effective Burgers vectors and lead to the formation of interesting nanostructures with large Eshelby twists. These large effective Burgers also unravel the mechanism of formation of nanopipes and micropipes with hollow cores and nanotubes with Eshelby twist in technologically important materials, which are needed for realizing a variety of advanced solid-state devices ranging from light emitting diodes to high-frequency and high-power devices.\(^30,31\)

The role of screw of screw dislocations in crystal growth is quite pervasive across the scale from nanoscale to mesoscale. The chiral shapes in tellurium nanostructures are found to result from screw-dislocation-mediated growth. The handedness (left or right) of the shape seems to be dictated by screw dislocations. Screw dislocations within the seed during crystal growth can also provide a template for spiral self-organization and the growth of metastable phases. In MgZn\(_2\), the metastable Laves phase was found to nucleate from the liquid, with screw dislocations that intersected solid—liquid interfaces, thus catalyzing the spiral growth of the two-phase microstructure.\(^26\) In view of the formation of defect-mediated helical dislocations and double helices, it should be interesting to see how the helicity of a screw dislocation affects the chirality of grown crystals and the formation of novel metastable phases. Thus, the discovery of double helix of screw dislocations stands to impact our understanding of crystal growth and the formation of crystalline structures across the nanoscale to mesoscale for next-generation solid-state devices.

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**Notes**

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