The hardness of nanotwinned diamond (nt-diamond) is reported to be more than twice that of the natural diamond, thanks to the fine spaces between twin boundaries (TBs), which block dislocation propagation during deformation. In this work, we explore the effects of additional TBs in nt-diamond using molecular dynamics (MD) calculations and introduce a novel intersectional nanotwinned diamond (int-diamond) template for future laboratory synthesis. The hardness of this int-diamond is predicted by first analyzing individual dislocation slip modes in twinned grains and then calculating the bulk properties based on the Sachs model. Here we show that the hardness of the int-diamond is much higher than that of nt-diamond. The hardening mechanism of int-diamond is attributed to the increased critical resolved shear stress due to the presence of intersectional TBs in nt-diamond; this result is further verified by MD simulations. This work provides a new strategy for designing new super-hard materials in experiments.

RESULTS
Dislocation slip modes in int-diamond grains
For diamond, dominant dislocations are along the <110> directions slipping in the (111) plane with Burgers vector of \( \frac{1}{2} <110> \) for perfect dislocation and \( \frac{1}{2} <112> \) for glide-set partial dislocation \(^{14}\). According to the angle between Burgers vector and dislocation line direction, there are six types of dislocations: glide-set 0° perfect dislocations, glide-set 30° partial dislocations, glide-set 60° perfect dislocations, glide-set 90° partial dislocations, shuffle-set 0° perfect dislocations, and shuffle-set 60° perfect dislocations \(^{14}\). Among them, shuffle-set 0° perfect dislocation has the lowest critical resolved shear stress (CRSS) for dislocation motion and the lowest barrier strength when reacting with TBs \(^{14}\).

Here the CRSS is defined as the threshold stress of dislocation motion, and the barrier strength is defined as the threshold stress of dislocation reaction with the TB when the activation energy reaches zero \(^{19}\). Therefore, at room temperature, the hardness of the diamond is primarily controlled by the behavior of shuffle-set 0° perfect dislocations \(^{16,20}\). Therefore, in the present study, the hardness of the int-diamond will be analyzed based on the behavior of shuffle-set 0° perfect dislocations.

In an int-diamond grain, two different orientation twin boundaries TB1 and TB2 coexist and interweaved, whose average twin thickness is \( \lambda_1 \) and \( \lambda_2 \), respectively (Fig. 1a) \(^{21,22}\). TB1 and TB2 segment the grain into domains with four different crystallographic orientations, that is, orientations D1, D2, D3, and D4. Among these different orientations, lattices of D1 and D3, and D2 and D4 are mirror images across TB1 and TB2, respectively. Consequently, the slip systems in an int-diamond grain can be expressed by a combination of four Thompson tetrahedra (in Fig. 1b): ABCD, ABCD1, A'B'C'D', and A'B'C'D'1, which correspond to D1, D2, D3, and D4, respectively.
The combination of these four Thompson tetrahedra results in 39 slip systems in an int-diamond grain (Table 1). According to dislocation line directions and their slip plane orientations, the slip modes of shuffle-set 0° perfect dislocations in int-diamond are divided into four types: slip transfer (ST) mode, confined layer slip (CLS) mode, confined slip transfer mode I (CST-I) and confined slip transfer mode II (CST-II) modes, all of which are schematically plotted in Fig. 1b. For ST mode, the slip planes are parallel to either TB1 or TB2, and the respective dislocation lines are located within either TB5 or TB1. For CLS mode, the slip planes are parallel to either TB1 or TB2, while the respective dislocation lines are non-parallel to TB2 or TB1. For CST-I mode, both slip planes and dislocation lines are non-parallel to any TB. For CST-II mode, the slip planes are non-parallel to any TB, while the respective dislocation lines are located within either TB1 or TB2. As a result, the interactions of these slip modes with TBs are different. This leads to different CRSSs for the four slip modes. For ST mode, the dislocation-TB reaction is characterized by dislocations propagating within the TBs and the corresponding CRSS is determined by the lattice frictional stress and barrier strength of shuffle-set 0° perfect dislocations reacting with the TBs. For CLS mode, the dislocation motion is confined between two TBs and its CRSS can be evaluated by increased dislocation energy due to the dislocation line left on the two TBs. For CST-I mode, the shuffle-set 0° perfect dislocation is confined between two TBs and then becomes shuffle-set 60° perfect dislocation to parallel TB when it reaches TB because the initial dislocation line is non-parallel to TB. Finally, the shuffle-set 60° perfect dislocation interaction with TB to propagate through TB, and its CRSS is determined by the barrier strength of shuffle-set 60° perfect dislocations reacting with TBs and increased dislocation energy because produced dislocation on two TBs. For CST-II mode, although its dislocation motion is similar to that in CST-I mode, its barrier strength is determined by shuffle-set 0° perfect dislocations reacting with the TB. In order to obtain CRSSs for these slip modes, barrier strengths of shuffle-set 0° and 60° perfect dislocations reacting with TBs must be calculated first. Barrier strengths of dislocation reaction with TB

Shuffle-set 0° and 60° perfect dislocations reacting with TBs can be considered as a kink nucleation and migration process (Fig. 1c and Supplementary Fig. 1). The shear-stress dependent activation energy for kink nucleation and migration are calculated (detail in “Methods” section), and the results are plotted in Fig. 1d. With increasing shear stress, the activation energies for shuffle-set 0° and 60° perfect dislocations reacting with TB reach zero at shear stresses of 19 and 48 GPa, respectively. These stresses are considered the respective barrier strengths for shuffle-set 0° and 60° perfect dislocations. The twin intersecting points can provide the pinning obstacle for the slip of dislocation when the shuffle-set dislocation slip along the twin plane. However, in nt-diamond, the shuffle-set dislocations slip along twin plane energetically show no advantage over those along other slip planes. Therefore, the shuffle-set dislocation is favor to slip along the slip planes rather than twin plane, and the pinning effect of intersecting points on shuffle-set dislocation motion is neglected in this work.

CRSS for ST mode

In ST mode, dislocation motions are blocked by TBs (inset of Fig. 2a). According to dislocation pile-up theory, the CRSS (τ_{css}) of this mode is expressed as the following:

\[ \tau_{css}^{ST} = \tau_0 + \left( \frac{\tau_B G b}{\pi \lambda} \right)^{1/2}, \]

where \( \tau_0 \) is lattice frictional stress; \( G \) is the shear modulus; \( b \) is the magnitude of the Burgers vector; \( \lambda \) is twin thickness of
Table 1. Slip system categories in int-diamond.

| No. | Category | Slip system | Slip plane | Direction |
|-----|----------|-------------|------------|-----------|
| 1   | ST mode  | DBC         | BC         | BC        |
| 2   | ABC      | BC          |            |           |
| 3   | A’BC     | BC          |            |           |
| 4   | D’BC     | BC          |            |           |
| 5   | A’BC     | BC          |            |           |
| 6   | CLS mode | DBC         | DB         |           |
| 7   | DBC      | DB          |            |           |
| 8   | D’BC     | D’C         |            |           |
| 9   | A’BC     | A’B         |            |           |
| 10  | A’BC     | A’C         |            |           |
| 11  | A’BC     | A’B         |            |           |
| 12  | A’BC     | A’C         |            |           |
| 13  | ABC      | AB          |            |           |
| 14  | ABC      | AC          |            |           |
| 15  | ABC      | AB          |            |           |
| 16  | CST-I mode | DAB      | AD         |           |
| 17  | A’DB     | A’D         |            |           |
| 18  | D’AB     | A’D         |            |           |
| 19  | A’D’B    | A’D’        |            |           |
| 20  | DAC      | AD          |            |           |
| 21  | A’DC     | A’D         |            |           |
| 22  | D’AC     | A’D         |            |           |
| 23  | A’D’C    | A’C         |            |           |
| 24  | CST-II mode | DAB  | AB         |           |
| 25  | A’DB     | A’B         |            |           |
| 26  | D’AB     | AB          |            |           |
| 27  | A’D’B    | A’B         |            |           |
| 28  | DAC      | AC          |            |           |
| 29  | A’DC     | A’C         |            |           |
| 30  | D’AC     | AC          |            |           |
| 31  | A’D’C    | A’C         |            |           |
| 32  | DAB      | DB          |            |           |
| 33  | A’DB     | DB          |            |           |
| 34  | D’AB     | D’B         |            |           |
| 35  | A’D’B    | D’B         |            |           |
| 36  | DAC      | DC          |            |           |
| 37  | A’DC     | DC          |            |           |
| 38  | D’AC     | D’C         |            |           |
| 39  | A’D’C    | D’C         |            |           |

CRSS for CLS mode

The CRSS for CLS mode can be calculated on the basis of the virtual work principle (Eq. 2), and it is expressed as: refs. 25,26

$$r_{CLS}^{CSS} = \tau_0 + \frac{Gb(1 - \nu \cos^2(\phi) \sin \theta)}{2\pi(1 - \nu)} \frac{\lambda^2}{\ln B}$$

where \(\theta\) is the angle between the slip plane and the twin plane and \(\lambda\) is twin thickness; \(\nu\) is Possion ratio; \(\phi\) is the angle between the dislocation line and the Burgers vector, \(a\) is dislocation core parameter.

With the corresponding parameters from ref. 14 and materials parameters of the diamond (listed in Supplementary Table 1), the CRSS for CLS mode is expressed as:

$$r_{CLS}^{CSS} = 10.3 + 22.1 \lambda \ln \left( \frac{3.33\lambda}{0.25} \right).$$

Using Eq. 4, the CRSS for CLS mode is calculated and plotted in Fig. 2a. This CRSS increases with decreasing twin thickness, and the values are similar to that of CLS mode in nt-diamond.

CRSS for CST-I mode

In CST-I mode, dislocation motions are confined by TB1 or TB2 and blocked by TB1 or TB2, respectively. Therefore, the corresponding CRSS is affected by both the Hall–Petch effect and the confined intersectional twin; \(r_{TB} = 19\) GPa as calculated above and \(\tau_0 = 10.3\) GPa (see “Methods” section) and assuming \(\lambda_1 = \lambda_2 = \lambda\), twin thickness-dependent CRSS for ST mode is rewritten as the following:

$$r_{ST}^{CSS} = 10.3 + 28\lambda^{1/2},$$

which is plotted in Fig. 2a. This CRSS increases with decreasing twin thickness, and the trend and quantitative values are similar to that of ST mode in nt-diamond.
The resulting CRSS as a function of twin thickness is plotted in Fig. 2b. Due to the lower barrier strength of shuffle-set 0° perfect dislocations reacting with TB, the CRSS is smaller than that of CST-I at the same twin thickness. Owing to the combined Hall–Petch and confined layer slipping effects, this CRSS is also higher than that of ST and CLS modes at the same twin thickness.

Hardness of bulk int-diamond based on the Sachs model

The Sachs model is a single-slip system model for mechanical properties of polycrystalline materials, and it is a particularly effective method to investigate the yield strength of polycrystalline materials with anisotropic slip systems17. For int-diamond, dislocations in multiple twin domains change directions and slip planes in such complex manner (as shown in Figs. 1 and 2) that the CRSS is affected by both the Hall–Petch effect and the confined layer slipping effect; therefore, the CRSS for CST-II can be expressed by Eq. 5. The difference is that in this case, τfl refers to the barrier strength of shuffle-set 0° perfect dislocations reacting with TB. Based on Eq. 5 and the parameters of the diamond, the CRSS for CST-II mode is expressed as:

\[
\tau_{css}^{CST-II} = 10.3 + 28\lambda^{-1/2} + 22\frac{\ln(3.33\lambda)}{\lambda}. \tag{7}
\]

The CRSS of CST-II mode thus calculated is plotted in Fig. 2b. Due to the lower barrier strength of shuffle-set 0° perfect dislocations, the CRSS is smaller than that of CST-I at the same twin thickness. Owing to the combined Hall–Petch and confined layer slipping effects, this CRSS is also higher than that of ST and CLS modes at the same twin thickness.

Verification of int-diamond hardness by MD simulation

To further confirm the calculated results by Sachs model, the yield strength of polycrystalline int-diamond is studied by using MD simulation. The calculated stress-strain curve of the int-diamond is plotted in Fig. 4. The yield strength is equal to 165 GPa for int-diamond, 154 and 161 GPa for nt-diamond at twin thickness of 5.5 and 1.2 nm, and 140 GPa for ng-diamond, respectively. Although the strain rate (5 × 10^8 s^-1) in MD simulation is higher than that of the experiment, these results qualitatively confirm that the yield...
Fig. 4 Calculated stress-strain curves of int-diamond, nt-diamond, and ng-diamond. The red, yellow, blue and cyan line is the stress-strain curve of int-diamond with twin thickness $\lambda_1 = 5.5$ nm and $\lambda_2 = 1.2$ nm, nt-diamond with twin thickness $\lambda$ of 5.5 and 1.2 nm, and ng-diamond, respectively.

The dislocation reaction with TB is a process of kink formation and migration, and the schematic for this process is plotted in insert of Supplementary Fig. 2. To simulate this process, a diamond structure model was built first. In this model, its $x$, $y$, and $z$ axis are along the $[112]$, $[\bar{1}10]$, and $[111]$ direction, the dimensions of $x$, $y$, and $z$ axis are 20.9, 2.5, and 13.8 nm, respectively, and contains about 120000 carbon atoms. Next, a series of kinked shuffle-set 0° and 60° perfect dislocation with different kink pair widths was introduced in the twin plane located at the center of the diamond structure model. On the basis of these models, the shear stress dependent activation energy of shuffle-set 0° perfect dislocation slip in diamond is plotted in Supplementary Fig. 2. When the activation energy of the dislocation slip reaches zero, the corresponding shear stress can be considered as the lattice friction stress.

**DISCUSSION**

We have examined the mechanical properties of diamond with a novel microstructure by introducing intersectional twin boundaries in ng-diamond. A total of 39 slip systems in four slip modes of this designer diamond (int-diamond) are systematically determined. In this model, their $x$, $y$, and $z$ axis are along diamond matrix’s $[112]$, $[\bar{1}10]$, and $[111]$ directions, the dimensions of $x$, $y$, and $z$ axis are 20.9, 2.5, and 13.8 nm, respectively, and contains about 120000 carbon atoms. Next, a series of kinked shuffle-set 0° and 60° perfect dislocation with different kink pair widths was introduced in the twin plane of the cuboid diamond twin structure model by using dislocation displacement field method (in Supplementary Fig. 1).

MD simulations were then performed by using LAMMPS program, and C–C bonding interactions were described by LCBOP potential. Periodic boundary condition was only imposed along the $y$ direction and the free surface was imposed in $x$ and $z$ directions. All these constructed structures were relaxed via energy minimization under different shear stress conditions. After relaxation, kink width dependent system energies were obtained and the maximum excess energy can be considered as kink formation energy ($2E_f$) at given shear stress. At the same time, a kink migration energy ($E_m$) were calculated by using NEB method. Finally, the activation energy $Q$ of dislocation reaction with TB is obtained according to $Q = 2E_f + E_m$. The shear stress-dependent activation energy for dislocation reaction with TB is plotted in Fig. 1d. As shown in Fig. 1d, when the activation energy of dislocation reaction with TB reaches zero, the corresponding shear stress can be considered as the barrier strength for a dislocation reacting with TB.

**METHODS**

**Barrier strength**

The dislocation reaction with TB is a process of kink formation and migration, and it is schematically plotted in Supplementary Fig. 1. To simulate this process, a cuboid diamond twin structure model was first built. In this model, their $x$, $y$, and $z$ axis are along diamond matrix’s $[112]$, $[\bar{1}10]$, and $[111]$ directions, the dimensions of $x$, $y$, and $z$ axis are 20.9, 2.5, and 13.8 nm, respectively, and contains about 120000 carbon atoms. Next, a series of kinked shuffle-set 0° and 60° perfect dislocation with different kink pair widths was introduced in the twin plane of the cuboid diamond twin structure model by using dislocation displacement field method (in Supplementary Fig. 1). MD simulations were then performed by using LAMMPS program, and C–C bonding interactions were described by LCBOP potential. Periodic boundary condition was only imposed along the $y$ direction and the free surface was imposed in $x$ and $z$ directions. All these constructed structures were relaxed via energy minimization under different shear stress conditions. After relaxation, kink width dependent system energies were obtained and the maximum excess energy can be considered as kink formation energy ($2E_f$) at given shear stress. At the same time, a kink migration energy ($E_m$) were calculated by using NEB method. Finally, the activation energy $Q$ of dislocation reaction with TB is obtained according to $Q = 2E_f + E_m$. The shear stress-dependent activation energy for dislocation reaction with TB is plotted in Fig. 1d. As shown in Fig. 1d, when the activation energy of dislocation reaction with TB reaches zero, the corresponding shear stress can be considered as the barrier strength for a dislocation reacting with TB.

**Lattice friction stress**

For shuffle-set 0° perfect dislocation slip in diamond, it also can be considered as a process of kink formation and migration, and the schematic for this process is plotted in insert of Supplementary Fig. 2. To simulate this process, a diamond structure model was built first. In this mode, its $x$, $y$, and $z$ axis are along the $[112]$, $[\bar{1}10]$, and $[111]$ direction and with dimensions of 20.9, 2.5, and 13.8 nm, respectively. Then, a series of kinked shuffle-set 0° perfect dislocation with different kink pair widths were introduced in the slip plane located at the center of the diamond structure model. On the basis of these models, the shear stress dependent kink formation and migration energy is obtained by adding shear stress to the diamond structure model by using the method as described above (methods section of Barrier strength). Finally, the shear stress-dependent activation energy of shuffle-set 0° perfect dislocation slip in diamond is plotted in Supplementary Fig. 2. When the activation energy of the dislocation slip reaches zero, the corresponding stress is the lattice friction stress.

**int-diamond hardness by using Sachs model**

Sachs model is an effective method to investigate the yield strength for polycrystalline materials with anisotropic slip system. In Sachs model, the yield strength of each grain can be expressed as:

$$\sigma_m = \min(n \sigma_{m}^{i}, \sigma_{m}^{ii}, \sigma_{m}^{iii}, \sigma_{m}^{g})$$

where $\sigma_{m}^{i}$ represents the yield strength of $m$-th slip system in $n$-th grain and it can be expressed as following:

$$\sigma_{m}^{g} = \frac{R_{CRSS}^{m}}{\mu_{m}}$$

where the $R_{CRSS}^{m}$ is the CRSS of $m$-th slip system; $\mu_{m}$ is the Schmid factor of $m$-th slip system in $n$-th grain.

In this work, a polycrystalline model with 6000 random orientations grains is considered. The yield strength for each grain can be obtained by using Eqs. 8 and 9. On the basis of these critical yield strength, we determine whether the grain yielded under a given uniaxial stress condition. As shown in Fig. 3a, the fraction of yielded grains increased with increasing uniaxial stress, when the fraction of yielded gain reaching 90%, the corresponding stress can be considered as the yield strength for this polycrystalline material. Further its hardness can be obtained by tripling its yield strength.

**MD simulation method for yield strength calculation**

In this work, atomic models for int-diamond, nt-diamond, and ng-diamond were constructed by using Voronoi polyhedron method. As shown in Supplementary Fig. 3, each model contain 20 grains with an average grain size of 16.23 nm. For int-diamond model, the twin boundaries TB, have two types: $\Sigma=27(115)$ and twin boundary TB, is $\Sigma=111$. In this structure model, the fraction of twin boundary $\Sigma=111$ is ~75%, and the fraction of twin boundary $\Sigma=111$ can be further...
improved to asymptotically approach unity\cite{65}. The twin thickness is 5.5 nm for TB1, and 1.2 nm for TB2. In the nt-diamond model, the twin thickness is 5.5 and 1.2 nm.

The MD simulations were then performed on these atomic models by using the popular LAMMPS code\cite{41}, and atomic configurations were visualized and analyzed by using the OVITO package\cite{46}. In this MD simulation, the C–C bonding interactions were described by Tersoff potential\cite{47} and the isothermal–isobaric (NPT) scheme was used\cite{48}. The time-step is set as 0.001 ps, relaxation time is 200 ps. After structure optimization under 300 K and ambient pressure, the compressive deformation is applied along x direction under a constant strain rate of $5 \times 10^{-5}$ s$^{-1}$ with a total true strain of 0.3, and the corresponding stress-strain curves were recorded. The maximum stress in the recorded stress-strain curves can be considered as the corresponding yield strength.

**DATA AVAILABILITY**

The authors declare that the data supporting the findings of this study are available within the paper and its Supplementary Information files.

**CODE AVAILABILITY**

All atomic simulations were performed by using the open source LAMMPS code\cite{41}.

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COMPETING INTERESTS
The authors declare no competing interests.

ADDITIONAL INFORMATION
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