Glide Mobility of a-Type Edge Dislocations in Aluminum Nitride by Molecular Dynamics Simulation

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ABSTRACT: Classical molecular dynamics simulations are performed to investigate the motion of a-type edge dislocations in wurtzite aluminum nitride (AlN). The nucleation and propagation of kinks are observed via the dislocation extraction algorithm. Our simulation results show that the nucleation energy of the kink pair in AlN is 1.2 eV and that the migration energy is 2.8 eV. The Peierls stress of the $1/3\langle1120\rangle\{1010\}$ edge dislocation at 0 K is 15.9 GPa. The viscous motion of dislocations occurs when $\tau > \tau_p$, and the dislocation velocity is inversely proportional to the temperature and directly proportional to the applied stress. Below room temperature, the value of the critical resolved shear stress (CRSS) on the prismatic plane is the lowest, which suggests that the dislocation mobility on the prismatic plane is the easiest. The CRSS on the pyramidal plane is always the highest at all temperatures, which suggests that pyramidal slip is the hardest among these three slip systems.

1. INTRODUCTION

The III-V semiconductor AlN has received considerable attention because of its outstanding properties in terms of physics and mechanics, such as high thermal conductivity, excellent electrical insulation, wide direct electronic energy band, and high bending strength.\textsuperscript{1,2} Intense research efforts have been devoted to studying AlN applications in electronic circuit components, optoelectronics, and power semiconductor devices.\textsuperscript{3}

Some results show that defects have great influence on the electrical and optical properties of AlN crystals.\textsuperscript{4,5} Numerous studies have been developed to reduce dislocations and comprehend the mechanisms of dislocation nucleation and motion. Although the physical vapor transport (PVT) AlN single-crystal growth method has reduced the dislocation density to a certain extent,\textsuperscript{6-9} thousands of dislocations still exist in AlN substrates. Questions about the structure of AlN dislocation cores and entanglement mechanisms that may impede further reduction remain. Thus, a direct calculation of the dislocation mobility is necessary for potential applications in crystal plasticity.

The AlN crystal structure is a well-known wurtzite-type structure with lattice parameters of $a = 0.311$ nm, $c = 0.498$ nm, and $c/a = 1.6$.\textsuperscript{10} Experimental studies have shown that most threading dislocations are perfect edge dislocations.\textsuperscript{11,12} They have Burgers vector $b = a/3\langle1120\rangle$ and slip on the $\{0001\}$, $\{10\bar{1}0\}$, and $\{10\bar{1}1\}$ planes. They are labeled as basal dislocations, prismatic dislocations, and pyramidal dislocations. It was pointed out that dislocation mobility is strongly influenced by the core structure.\textsuperscript{13} For covalently bonded materials, strongly directional atomic bonds induce high Peierls stress and a very narrow dislocation core. Not only analyses but also some attempts were made to manipulate the dislocation mobility.\textsuperscript{14} In some semiconductor crystals, a drastic increase of the dislocation velocity is observed during electronic excitation. A steep decrease in hardness indicates the beginning of macroscopic dislocation motion and plastic deformation. The hardness of AlN and GaN single crystals, which belong to the same group of III-V compound, decreases as the temperature increases. When temperatures are higher than $(1/2-2/3) T_m$ ($T_m$ is the melting point), plastic deformation rather than brittle fracture occurs in the semiconductor crystals. For a dislocation to glide, the value of the critical resolved shear stress should be higher than the yield stress. The yield stress of GaN is approximately 100–200 MPa even at 1000 °C.\textsuperscript{15}

In recent years, many atomistic studies have proven that dislocation mobility is affected by various external factors, such as stress and temperature.\textsuperscript{16,17} Dislocation velocity shows an increasing tendency as the stress is increased in the low-stress region.\textsuperscript{18} Under low temperature, the nucleation and propagation of the kink pair cause the mobility of the edge dislocation.\textsuperscript{13} Since kinks prefer to nucleate at higher
temperatures, the dislocations move fast by a kink-pair mechanism.\textsuperscript{19} Due to the covalency in the interatomic bonding and the different dislocation core structures, the dislocations in covalent crystals and metallic crystals are different in various respects;\textsuperscript{20} the former can produce deep energy levels in the bandgap and have more dislocation types. The dislocation mobility of these covalent crystals is controlled by the Peierls mechanism, and the mechanism of the dislocation glide in these covalent crystals is largely the same.

From an experimental point of view, the growth temperature of bulk AlN crystals by the PVT method is very high, its availability is very limited,\textsuperscript{20,21} and the deformation of AlN cannot be achieved at low temperature without pre-strain at high temperature. Therefore, physical experiments on AlN plasticity are difficult, and scant research on the precise mechanisms of the glide mobility of a-type edge dislocations in AlN has been investigated. In this work, molecular dynamics simulations are performed to obtain the nucleation and propagation of the kink pair. The Peierls stress at 0 K of the 1/3⟨1120⟩{1010} edge dislocation is calculated based on the obtained stress–strain curve. Finally, the effects of temperature and external applied stress on CRSS and dislocation velocity are explored.

### 2. SIMULATION METHOD

There are a number of interatomic potentials available for AlN, such as Tersoff potential, Vashishta potential, and SW potential. They are typical semiempirical potentials for simulating the Peierls stress and dislocation mobility. All of them can accurately capture a broad range of material properties, including cohesive energy, structure properties, and elastic constants.\textsuperscript{22} Tersoff potential is dependent on the bond order concept and can be generalized to handle mixed elements, which implies that it can reproduce the structural and mechanical properties of AlN. Vashishta potential has been used successfully for semiconductors and ceramic materials.\textsuperscript{23} Based on the Stillinger–Weber (SW) potential, Vashishta potential combines repulsive, screened charge-dipole, screened Coulombic, and dispersion interactions with bond-angle energy. Xiang et al.\textsuperscript{10} have compared the mechanical and physical properties of AlN with different interatomic potentials to explore their validity, availability, and accuracy in MD simulations. In this work, the Tersoff potential is chosen since it can provide good agreement with the DFT calculations.\textsuperscript{24,25} The optimized parameters in Tersoff potential suggested by Tungare et al.\textsuperscript{26} and Xiang et al.\textsuperscript{10} are employed. Simulations of dislocations are performed using the molecular dynamics LAMMPS code.\textsuperscript{27} As illustrated in Figure 1, to simulate dislocation motion, we follow the method described by Lunev et al.,\textsuperscript{28} wherein the initial cell is created from two half-crystals referred to as the “lower” and “upper” crystals. The size of the simulation cell might affect the dislocation velocity. In this work, the 58b × 24b × 48b simulation cell contains around 0.27 million atoms (b is the length of the Burgers vector). Our investigation as well as literature studies by Monnet and Terentiev\textsuperscript{29} and Murphy et al.\textsuperscript{30} shows that this cell size is adequate for eliminating the boundary effects on the strain field of a dislocation. The 1/3⟨1120⟩ direction (along the Burgers vector b) is parallel to the x axis of the cell, the 0001 direction (along the dislocation line) is parallel to the y axis, and the 1/3⟨100⟩ direction (orthogonal to the slip plane) is parallel to the z axis. Here, periodic boundary conditions are used along the x and y axes. However, a nonperiodic boundary condition is used along the z axis to ensure that a single dislocation is created. A fixed z boundary condition is used that leads to the formation of a single dislocation in the center instead of two opposite dislocations.

After energy minimization is performed with conjugate gradient relaxation,\textsuperscript{31} the system reaches convergence with an error tolerance at \(10^{-12}\). The dislocation core region is identified by applying common neighbor analysis.\textsuperscript{32} The dislocation segments illustrated in Figure 1 are identified with a dislocation extraction algorithm (DXA) in the subsequent simulation.

As shown in Figure 1, the dislocation mobility is simulated by applying external shear stresses to each atom in the upper and lower buffer layers along –x and x directions. The magnitude of the applied force is defined as \(\tau_{xx}(t) \cdot (L_x \cdot 1)/N\), where the applied shear stress is set to a ramp function, \(\tau_{xx}(t)\), which increased from zero to the maximum target value \(\tau_{xx}\) in the t ramp interval, and N is the total number of atoms contained in the buffer layer.

To avoid the thermal stress, the system relaxation is performed with molecular dynamics using an isothermal (NVT) ensemble. This procedure is repeated until the normal stresses near zero. After the relaxation, simulations are carried out using an adiabatic (NVE) ensemble, which were initiated with different temperatures T and shear stresses \(\tau\). A Langevin thermostat is chosen to keep the calculation at a prescribed temperature, and the time step of simulations is 1 fs. All these thermostat atoms and their motion are governed in Newton’s second law.\textsuperscript{33}

### 3. RESULTS AND DISCUSSION

#### 3.1. Stress and Displacement Fields in an Infinite Medium

As the dimension of a body containing a dislocation increases, stresses caused by surface boundary conditions decrease, and the stress field approaches that of a dislocation in an infinite medium. This stress field is termed the self-stress of the dislocation. The self-stress exerts no force on a dislocation in an infinite, homogeneous body. However, thermodynamic forces are introduced by free surfaces or internal surfaces, as well as any sources of stress that are superposed onto the self-stress.

The stress–field characteristic of the edge dislocation is determined from the differential equation for the Airy stress
function,\textsuperscript{34} which furnishes the stress components in Cartesian coordinates. Figure 2 presents simple diagrams of the stress distribution around an edge dislocation. The self-stress of an edge dislocation is antisymmetric and therefore does not produce a thermodynamic force on the dislocation.

3.2. Kinks on the $\frac{1}{3}(1120)\{1010\}$ Edge Dislocation. It is known that there are two sequential processes for a dislocation to move across the Peierls potential: the nucleation and migration of the kink pair.\textsuperscript{35} At finite temperature, edge dislocations move primarily through the nucleation and propagation of the kink pair. The value of the critical resolved shear stress decreases with increasing temperature, which can be explained by this mechanism.\textsuperscript{36} Furthermore, we consider the kinks’ mechanism to reasonably describe the evolution of dislocation mobility with temperature. We calculate the nucleation and migration energies of the kink pair on the $\frac{1}{3}(1120)\{1010\}$ edge dislocation. The thermally activated dislocation mobility is controlled by kinks extended over the Peierls valley. We obtain the evolution of CRSS and dislocation mobility with temperature by using the kink-pair nucleation model in the next section.

3.2.1. The Kink-Pair Nucleation Mechanism of Edge Dislocation Motion. Thermally activated dislocation mobility is determined by the probability (per unit time per unit length of a dislocation) of kink-pair nucleation. As shown in Figures 3 and 4, the width of a kink is approximately $b - 2b$, where $b$ is the length of the Burgers vector. It is easier for edge dislocations to move along the Burgers vector than along the dislocation line. According to the theory of dislocation mobility with various temperatures and shear stresses created by Hirth and Lothe, the kink-pair formation mechanism is used to analyze the shape of the dislocation line. Each kink contains a negative and a positive kink. Normally, on the adjacent Peierls valleys, the dislocation segments are connected by kinks.

The motion of a dislocation line is determined with two modes: the kink chain mode and the continuous vibrating string mode. As shown in Figure 3, when $T = 500$ K, the diffusion velocity is small, so that the dislocation segment reaches equilibrium and a kink chain will be formed. In this mode, the dislocation segments are gradually displaced by the motion of the kink pair, and the line tension is minimized. On the Peierls valley, the carrier of dislocation segments is the kink, which is unstable and easy to collapse. The rate of kink-pair nucleation $J$ increases when the temperature rises to 2000 K (Figure 4), and the dislocation line is considered to be a continuous vibrating string instead of a kink chain. As shown in Figure 4, kinks may span several valleys at high temperatures.

3.2.2. The Nucleation and Migration Energies of the Kink Pair. The nucleation and migration energies of the kink pair are calculated by the following formulae:\textsuperscript{35}

$$E_n = E_{KP} - E_{ED}$$  \hspace{1cm} (1)

$$E_m = \frac{\sum_{i=1}^{N} (E_{in} - E_{io})}{N}$$  \hspace{1cm} (2)

where $E_n$ and $E_m$ represent the nucleation and migration energies of the kink-pair. $E_{ED}$ is the total energy of the edge dislocation system, and $E_{KP}$ is the energy of the subsequent kink-pair system. $E_{in}$ is the total energy of systems when the $i$th atom is at the saddle point. $E_{io}$ is the total energy of systems
performing calculations on a simulation cell of height close to
determine the migration energy of both K⁺ and K⁻ kinks by
labels these migrating atoms and do further calculations. We
dislocation core atoms on the kink pair differ from all other atoms by their relatively large
centro-symmetry-deviation parameter, based on which we can
ter from all other atoms by their relatively large
increment. Figure 5 shows the corresponding stress–strain
curve. It is observed that the strain increases linearly with stress
until it equals the Peierls of 15.9 GPa. Then, the calculated
stress is close to constant since the dislocation glide releases
the excessive induced stress.

3.3.2. Evaluation of Dislocation Velocity. According to the
theory of dislocation motion, two modes of dislocation motion are
determined by various mechanisms in perfect crystal lattice
semiconductors. The first is the viscous motion that is shown
in Figure 6 region III. In this region, with \( \tau > \tau_p \), the dislocation velocity \( V \) is expressed by the following equation:

\[
V = \frac{tb}{B(T)}
\]

where \( B(T) \) is the dynamical drag that is proportional to the
temperature \( T \); so the dislocation velocity \( V \) increases with the
acting force \( \tau \) and decreases with the temperature \( T \). The
second is the thermally activated mode with \( \tau \leq \tau_p \), in which
the dislocation motion occurs via the thermally activated
nucleation and migration of the kink pair (shown in Figure 6
regions I and II). The dislocation glide in this region at low
temperatures is controlled by the Peierls mechanism, which
contains three processes: the formation of the kink pair, the
migration of the kink pair along the dislocation line, and the
annihilation or arrival of kinks at the end of the dislocation
line. The velocity of dislocation can be described by
dislocation motion modes. A dislocation motion model
developed by Hirth is used to obtain the Peierls stress. This
model has been used to estimate the Peierls stress of
semiconductor materials such as Si and SiGe.

3.3.1. Dislocation Motion at 0 K. The molecular dynamics
method is used to simulate the motion of the 1/3{11\( \overline{2} \)0}{10\( \overline{1} \)0} dislocation at 0 K. The dislocation model is
set up following the method described in part two: The
periodic boundary conditions are applied along the \( x \) and \( y \)
axes. The dislocation line is along the \( y \) axis. With the
introduction of an elastic strain (\( xz \)-tilt), the shear stress on the
 glide plane increases gradually. The strain is increased by 0.1% per
step and an energy minimization is performed after each increment. Figure 5 shows the corresponding stress–strain

Figure 4. Thermally activated motion of edge dislocations at \( T = 2000 \) K. (a) Strongly bent dislocation line extending over two Peierls
valleys with double kinks at \( x = 4b - 3b \) and \( x = 3b - 2b \). (b) Dislocation segments at \( x = 2b \) progress to \( x = b \), while segments at \( x = b \) are pulled to \( x = 0 \).

Figure 5. Stress–strain curve at 0 K for the 1/3{11\( \overline{2} \)0}{10\( \overline{1} \)0} edge
dislocation.

3.3. Dislocation Motion in AlN Crystals. The mechanism
of the kink-pair motion is described with several
regions is shear stress by calculating the slope of displacement and time. Since the dislocation core. Finally, the dislocation velocity is measured in Table 1 is proposed by Yonenaga et al.43 The thermally activated regimes of dislocation motion can be defined as the core region of the edge dislocation. Then, the kink-pair nucleation rate \( \frac{J_{fi}}{h} \) is defined as the stress at which the dislocation velocity is 0.1 \( \overline{112} \) \{1100\} slip system. We choose the molecular dynamic range of a-type edge dislocations in wurtzite GaN using molecular dynamics. Chakraborty et al.44 described three virtual experimental methods to evaluate the CRSS of different slip systems in hexagonal materials. We simulate the deformation process and derive the velocities obtained in this paper are in the same order of magnitude with those of Weingarten and Chung,15 who had calculated the velocities of the three types of a-type edge dislocations in wurtzite GaN using molecular dynamics.

3.3.3. Critical Resolved Shear Stress (CRSS). It is important to understand the critical resolving shear stress of different slip systems to further simulate the plastic deformation of hexagonal materials. Chakraborty et al.44 described three virtual experimental methods to evaluate the CRSS of different slip systems in hexagonal materials. We choose the molecular dynamics method proposed by Fan et al.,36 and the CRSS is defined as the stress at which the dislocation velocity is 0.1 km/s. We simulate the deformation process and derive the data from the stress–strain curves.
The curves of CRSSs with temperature for different slip systems are presented in Figure 8. Significant variations in the CRSS values are evident in different slip systems. The value of CRSS on the prismatic plane ranges from 20 GPa to 844 MPa. The value of CRSS for the basal plane is apparently higher than that for the prismatic plane. Among them, edge dislocation on the prismatic plane is the easiest to activate. These results are discussed further in the following section.

3.3.4. Discussion. The nucleation process of the kink pair found in the edge dislocation can be described as follows: First of all, the kink pair may nucleate with a very large stress; then, it moves to another kink. The subsequent annihilation results in the energy release, which is approximately twice as much as the formation energy. It can be deduced from section 3 that the formation energy of a kink is approximately 1.2 eV in the case of that the interaction energy and the formation entropy are neglected. This means that the annihilation energy is close to 2.4 eV. This energy consists of two parts, half of which dissipates into heat, causing an increase in atomic kinetic energy, while the other half leads to an increase in crystalline potential energy.

In section 3.3.3, we describe the thermally activated mobility of edge dislocations on different planes via the values of CRSS evolution with temperature. The results show that with increasing temperature, the value of CRSS for the prismatic plane decreases significantly until the temperature reaches 1600 K. The value of CRSS is between 15 GPa and 845 MPa when the temperature is 600−1600 K. The CRSS value at low temperatures is reduced due to changes in dislocation density and slip mechanisms. Meanwhile, the dislocation motion is achieved by the simultaneous nucleation and collision of several kink pairs on the dislocation line. In our model, CRSS values above 1600 K tend to be constant instead of decreasing. Above this temperature, the CRSS value is dependent on the microstructure of the whole dislocation rather than simply relating to the stress that is required to cause a single dislocation motion, since the mobility will not be controlled anymore by kink-pair nucleation and propagation but by phonon drag. In other words, the dislocation core may emit vacancies, which are considered to be strong obstacles for dislocation motion. It is considered that the plasticity of the AlN single crystal is determined by the thermally activated dislocation glide on the prismatic plane between 50 and 1600 K.

For the convenience of comparison, we put the CRSS values on these three edge dislocations together in Figure 8. The CRSS values decrease significantly below 1000 K. Then, the CRSS on the prismatic plane decreases continuously with increasing temperature until it approaches zero stress at approximately 1600 K and then fluctuates very little around this value. Similarly, the CRSS values on the basal and pyramidal planes are also observed to decrease to a minimum value at ~1600 K. Below room temperature, the CRSS value on the prismatic plane is the lowest, which suggests that the dislocation motion on the prismatic plane is the easiest, and slip predominately occurs on the prismatic plane at those temperatures. At 300 K, the CRSS values on the basal plane are relatively close to those on the prismatic plane. It should be noted that basal slip becomes intense at and above room temperature. At these temperatures, when edge dislocations are temporarily immobile, accounting for interactions with other dislocations or stuck by obstacles, they are inclined to transform onto basal planes due to thermal activation. This suggests that slip on the basal plane is probably predominant at room temperature, and it remains slightly more difficult than that on the prismatic plane. The CRSS values on the prismatic and basal planes are relatively close to each other at intermediate temperatures ranging from 1000 to 1600 K. The CRSS value on the pyramidal plane is always the highest at all temperatures. This suggests that pyramidal slip is definitely the hardest among these three slip systems. When activated, the pyramidal slip system is subjected to strong Peierls friction, which is probably the source of the high CRSS values, and the dislocations on this plane move slowly due to the kink-pair mechanism. It is concluded that prismatic slip dominates at low temperatures because the yield stress increases with decreasing temperature. Figure 8 shows that prismatic slip and basal slip contribute the most to plasticity, while pyramidal slip has little influence on plasticity.

4. CONCLUSIONS

The thermally activated mobility of the 1/3(1120)(1010) edge dislocation in AlN arises with kink-pair nucleation and propagation at lower temperatures, and a higher nucleation rate is observed at higher temperatures. The calculated migration energy is 2.8 eV, which is much higher than the nucleation energy of 1.2 eV. It means that the migration of the kink pair is much harder than the nucleation. The Peierls stress of the 1/3(1120)(1010) edge dislocation at 0 K is calculated with the MD method and is obtained via the stress−strain graph. The Peierls stress equals 15.9 GPa.

When \( \tau \leq \tau_p \), dislocation motion is caused by thermally activated nucleation and migration of kink pairs. The dislocation glide in this region at low temperatures is controlled by the Peierls mechanism that contains three processes: the formation of a kink pair, the migration of the kink pair, and the annihilation of two kinks or the arrival of kinks at the end of the dislocation line. The viscous motion of dislocations occurs when \( \tau > \tau_p \) and the dislocation velocity is inversely proportional to the temperature and directly proportional to the applied stress. We find that the dislocation
velocity decreases as the temperature increases. This phenomenon is more significant under low pressure. A fluctuation of the velocity versus temperature is observed, particularly at high temperatures.

The CRSS values on the three slip planes (⟨0001⟩ planes, ⟨1010⟩ planes, and ⟨1011⟩ planes) are summarized as a function of temperature for comparison. The difference of CRSS on the three planes is much smaller after the temperature increased to higher than 1600 K. Below room temperature, the CRSS on the prismatic plane is the lowest, which suggests that the dislocation motion on the prismatic plane is the easiest, and the slip mainly occurs on the prismatic plane at those temperatures. At 300 K, the CRSS on the basal plane is relatively close to the value on the prismatic plane. This would suggest that at room temperature, slip on the basal plane is probably also predominant. The CRSS values on the basal and prismatic planes are relatively close to each other at intermediate temperatures ranging from 1000 to 1600 K. The CRSS on the pyramidal plane is always the highest at all temperatures. This suggests that pyramidal slip is the hardest among these three slip systems.

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