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Inhomogenous Dislocation Nucleation Based on Atom Potential in Hexagonal Noncentrosymmetric Crystal Sheet *

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By introducing internal degree, the deformation of hexagonal noncentrosymmetric crystal sheet can be described by the revised Cauchy–Born rule based on atomic potential. The instability criterion is deduced to investigate the inhomogeneous dislocation nucleation behavior of the crystal sheet under simple loading. The anisotropic characters of dislocation nucleation under uniaxial tension are studied by using the continuum method associated with the instability criterion. The results show a strong relationship between yield stress and crystal sheet chirality. The results also indicate that the instability criterion has sufficient ability to capture the dislocation nucleation site and expansion. To observe the internal dislocation phenomenon, the prediction of the dislocation nucleation site and expansion domain is illustrated by MD simulations. The developed method is another way to explain the dislocation nucleation phenomenon.

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The development of structure in the nanometer scale is being intensively attempted with the advent of the microscopic process technology. Experiments can not be easily carried out to explore nano-scale structure mechanical properties, therefore the microscopic process simulation technology (MPST) is gradually focused on and studied by Liu *et al.*,^[1,2] Liu *et al.*^[3,4] and Miller *et al.*^[5] Their results indicate that mechanical deformation is the forming process of material internal defects, which is the typical dislocation. It is also a complicated problem to ascertain what makes the dislocation nucleation and dislocation expansion. Many researchers have thrown their research interests on these problems and many meaningful simulations have been carried out for homogeneous nucleation and inhomogeneous nucleation problems. Dislocation nucleation at defect, such as grain boundary, has been studied by Liu *et al.*^[1,2] Experimental work have revealed that dislocations are unstable, and dislocations can nucleate internal or on boundary for sub-micro crystal pillar under compression.

On homogeneous dislocation nucleation, Liu *et al.*^[6] extended material instability down to the atomic scale. Li *et al.*^[7] introduced the instability criterion to predict the nano-indentation-induced dislocation nucleation problem. In the framework of Acharya dislocation field theory, Miller *et al.*^[8] presented a stress-gradient-based criterion which could predict the dislocation nucleation site of nano-indentation problem. On inhomogeneous dislocation nucleation, Kitamura *et al.*^[9] presented the sufficiency of using continuum instability criterion to study the inhomogeneous atomic system dislocation nucleation. The deformation description of noncentrosymmetric crystal has been proposed by Zhang *et al.*,^[10] however few research works on dislocation nucleation problem, based on homogeneous and continuum assumption, have been studied.

In continuum level, the typical representative cell deformation description of crystal is based on the Cauchy–Born rule, A homogeneous deformed crystal on the typical cell level may undergo inhomogeneous deformation inside the cell. In order to introduce the Cauchy–Born rule to describe its deformation, the crystal sheet can be decomposed into two sub-lattices marked by A and B, as shown in Fig. 1. Every sub-lattice, which possesses centrosymmetry, has a triangular lattice structure. The method is called the revised Cauchy–Born rule. Here we give the definition of crystal sheet orientation angle θ , which is shown in Fig. 1. Thus the strain energy function method can be easily used to give an approximation, based on the Cauchy–Born rule or the revised Cauchy–Born rule.



Fig. 1. A schematic diagram of the atomic sheet hexagonal structure.

The obtained method of P-K2 stress and deformation description of atomic bond length are outlined. Let \boldsymbol{E} denote Green strain tensor on the continuum level, r_{ij}^0 be the un-stretched bond length and n_{ij}^0 be the unit vector in the initial bond orientation for

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atoms i and j at the state of equilibrium, r_{ij} and n_{ij} be the stretched bond length and unit vector in the deformed configuration, respectively. Let \mathbf{F} denote the uniform deformation gradient on the continuum level at an arbitrary point i in the sub-lattice A. Besides being subjected to the same deformation gradient \mathbf{F} , the sub-lattice B may also undergo a rigid body translation with respect to the sub-lattice A, which is denoted by ξ . The corresponding movements of sub-lattice A and B are written as

$$r_{ij} = \boldsymbol{F} \cdot r_{ij}^0, \quad r_{ij} = \boldsymbol{F} \cdot (r_{ij}^0 + \boldsymbol{\xi}).$$
(1)

After the deformation, the stretched length of bond i - j becomes

$$r_{ij}^{2} = \boldsymbol{r}_{1} \cdot \boldsymbol{r}_{1} = (\boldsymbol{r}_{0} + \boldsymbol{\xi}) \cdot \boldsymbol{F}^{T} \cdot \boldsymbol{F} \cdot (\boldsymbol{r}_{0} + \boldsymbol{\xi}),$$
$$r_{ij} = \sqrt{\boldsymbol{r}_{1} \cdot \boldsymbol{r}_{1}} = \sqrt{(\boldsymbol{r}_{0} + \boldsymbol{\xi}) \cdot (2\boldsymbol{E} + \boldsymbol{I}) \cdot (\boldsymbol{r}_{0} + \boldsymbol{\xi})}.$$
(2)

For convenience, the partial derivatives of atomic bond length over Green deformation tensor E are given by

$$\begin{aligned} \frac{\partial r_{ij}}{\partial E} &= \frac{1}{r_{ij}} \left(r_{ij}^0 \boldsymbol{n}_{ij}^0 + \boldsymbol{\xi}_i \right) \otimes \left(r_{ij}^0 \boldsymbol{n}_{ij}^0 + \boldsymbol{\xi}_i \right), \\ \frac{\partial r_{ij}}{\partial \boldsymbol{\xi}_i} &= \frac{1}{r_{ij}} \left(\boldsymbol{I} + 2\boldsymbol{E} \right) \cdot \left(r_{ij}^0 \boldsymbol{n}_{ij}^0 + \boldsymbol{\xi}_i \right) \\ &= \frac{1}{r_{ij}} \left(\left(\boldsymbol{I} + 2\boldsymbol{E} \right) r_{ij}^0 \boldsymbol{n}_{ij}^0 + \left(\boldsymbol{I} + 2\boldsymbol{E} \right) \boldsymbol{\xi}_i \right), \\ \frac{\partial^2 r_{ij}}{\partial E^2} &= -\frac{1}{r_{ij}^3} \left(r_{ij}^0 \boldsymbol{n}_{ij}^0 + \boldsymbol{\xi}_i \right) \otimes \left(r_{ij}^0 \boldsymbol{n}_{ij}^0 + \boldsymbol{\xi}_i \right) \\ &\otimes \left(r_{ij}^0 \boldsymbol{n}_{ij}^0 + \boldsymbol{\xi}_i \right) \otimes \left(r_{ij}^0 \boldsymbol{n}_{ij}^0 + \boldsymbol{\xi}_i \right), \end{aligned}$$
(3)

where \otimes denotes the dyad. For hexagonal crystal, a representative cell, surrounding every atom in the sub-lattice A, includes only three neighbor atoms in the sub-lattice B. In addition, the strain energy density function W of a typical cell becomes

$$W = \frac{1}{\Omega_0} \frac{1}{2} \sum_{j=1}^3 V(r_{ij}), \tag{4}$$

where Ω_0 is the 2D cell area in the initial configuration. For a given deformation gradient F (or equivalent Green strain E), the vector ξ , related to the rigid body translation between sub-lattices A and B, is determined by minimizing W with respect to ξ ,

$$\frac{\partial W}{\partial \xi} = 0. \tag{5}$$

Substituting Eqs. (3) and (4) into Eq. (5) yields

$$\sum_{1 \le j \le 3} \left[\frac{\partial W}{\partial r_{ij}} \frac{1}{r_{ij}} \left((\boldsymbol{I} + 2\boldsymbol{E}) r_{ij}^0 \boldsymbol{n}_{ij}^0 + (\boldsymbol{I} + 2\boldsymbol{E}) \boldsymbol{\xi}_i \right) \right] = 0.$$
(6)

From Eq. (6) the internal freedom ξ can be determined. The P-K2 stress can also be obtained through the derivative of strain energy density function W over

Green strain E. By Eqs. (3) and (5), the P-K2 stress can be written as

$$\boldsymbol{S} = \frac{dW}{dE} = \frac{1}{\Omega_0} \left\{ \sum_{i}^{3} \left[\frac{1}{2} \frac{\partial V}{\partial r} \right] \frac{(\boldsymbol{r} + \boldsymbol{\xi}) \otimes (\boldsymbol{r} + \boldsymbol{\xi})}{|\boldsymbol{r}|} \right\}.$$
(7)

Until now, it is indicated that a deformation gradient is loaded on a crystal sheet, consequently strain energy density function can be obtained through the bond potential energy changing.

To analyze the unstable state criterion, it is considered that an atomic system consists of N atoms at equilibrium state. For a given deformation gradient, the Helmholtz free energy H of the atomic system can be written as functions of every atom position coordinate vector and the Green strain,.^[18]

$$H = H(X, E), \tag{8}$$

where X is the state of current configuration. In fact, Eq. (8) is a general expression of the Helmholtz free energy. For an infinitesimal change of H, it can be written as

$$\Delta H = H(X, E) - H(0, 0).$$
(9)

Equation (9) can be always extended into Tayler series, and the form over three orders does not considered,^[9]

$$\Delta H = V(X) \left[S : E + \frac{1}{2}E : L : E \right].$$
(10)

In Eq. (10) P-K2 stress S is work-conjugated to Green strain E. L is a four-order elastic stiffness tensor. V is a typical cell volume for 3D (or area for 2D) change from initial configuration to current configuration. The total energy consists of the Helmholtz free energy H and the work done by the external loading W_0 . Thus the total energy can be written as

$$G = H - W_0. \tag{11}$$

It should be pointed out that we only consider the system under the static external loading. Taylor's series expansion of the total energy G in terms of infinitesimal change is

$$\Delta G = \Delta H - \Delta W, \tag{12}$$

the partial derivative of G over E can be expressed as

$$\frac{\partial G}{\partial E} = g(X), \quad g(X) = \frac{\partial H}{\partial E} - V(X)S.$$
 (13)

For the arbitrary equilibrium state, g(X) is equal to zero. For non-equilibrium state, g(X) can be written in the form

$$g(X) = V(X)B : E, \tag{14}$$

$$B_{ijkl} = L_{ijkl} - \frac{\partial S}{\partial E}.$$
 (15)

From Eqs. (14) and (13), the infinitesimal change of the total energy can be written as

$$\Delta G = g(X) : \Delta E + V(X)\Delta E : B : \Delta E$$

= (V(X)B : E + V(X)\Delta E : B) : \Delta E. (16)

For any given deformation field, infinitesimal deformation always makes the total energy decrease. The crystal sheet will lose its stability if there is a state $\Delta G = 0$ for any given infinitesimal deformation. This means that the crystal sheet can endure deformation without total energy increasing, meanwhile disorder atoms exist and dislocation nucleation occurs in the crystal sheet. Thus we can make the state $\Delta G = 0$ as stability criterion, which can be rewritten as

$$\Lambda = \det(A) = 0, \quad A = (B^T + B)/2.$$
(17)

Here we consider that in all deformation forms,^[18] B is a four order tensor, and A, which satisfies the Voigt symmetry, is the symmetric form of B. From Eq. (17), we can investigate the positive definition of A. Furthermore, if there is an field $\Lambda \leq 0$, we can consider that dislocations begin to nucleate in the field.



Fig. 2. Computation simulation procedure.

The simulation procedure is illustrated in Fig. 2. In every time increment, there is a loading increment input in ABAQUS/Explicit. The corresponding strain increment can be obtained by the constitutive relation coded in user subroutine VUMAT, which is illustrated in Fig. 2. To obtain the internal freedom in every time increment, Newton iteration method is employed into solving procedure. The simulation model is a quadratic crystal sheet with a unite edge length. It is uniformly divided by 100 elements. L-J potential,^[11] which is shown in Eq. (18), is adapted in the simulation.

$$V(r) = 4\varepsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^6 \right], \qquad (18)$$

where σ and ε are chosen as unit one respectively. Atomic bond length is 1.122σ at the state of equilibrium between two atoms. Every typical representative cell is composed of three atoms by Zhang.^[10] A atomic bond in the cell is along with the +x axial direction. The initial atomic bond direction is rotated anticlockwise from 0° to 30° , which is one fourth of a periodicity for hexagonal crystal. The response of a 2D plane crystal sheet under uniaxial tension is studied. Meanwhile, the strain-stress curves and the strain-stability factor Λ curves are shown in one map. The stress amplitude of dislocation nucleation can be determined by the strain-criterion curve from Fig. 3. In Fig. 3, we can observe that the stress amplitude increases as the loading strain increases, and Λ decreases as the loading strain increases. Investigating the distribution contours of Λ , it is implied that the dislocation nucleation point and domain, as shown in Fig. 4 and Fig. 5, respectively.



Fig. 3. Stress-strain curves and the strain- criterion Λ curves.



Fig. 4. Dislocation nucleation criterion contour with the crystal sheet 0° .

To observe the internal dislocation state, MD simulation is given for the hexagonal crystal under tension. In the simulation, Tersoff carbon potential^[12] is adopted. The simulation temperature is 1 K, model size is $12.5 \times 10.65 \times 3.35$ nm³ and the period boundary condition is given along the +Z and -Z directions. The tension is along the +X and -X directions. In the simulation, the stable configuration is obtained by total energy minimization using conjugate gradient method before loading. The total strain is 0.02 and the strain rate is in the order of $5 \times 10^8 \,\mathrm{s}^{-1}$, which is typically used for MD tension simulation. When dislocation nucleation occurs, the atom configuration is plotted in Fig. 6 and the disorder atoms are circled in white line. Potential evolution of the atomic system with the loading time is also plotted in Fig. 6. It is inferred that there are disorder atoms in the model with the appearance of potential curve jumping, which means that we can judge the disorder atoms appearance through the atomic system potential curve.



Fig. 5. Dislocation nucleation criterion contour with the crystal sheet 6° .



Fig. 6. MD simulation internal microstructure of hexagonal crystal und tension.

Recently, the anisotropy of graphitic sheet and CNT under tension is focused by Chang *et al.*^[13] and Goze $et \ al^{[14]}$ Their results illustrate that Young's modulus for armchair tube is slightly larger than that for zigzag tube for a given tube diameter. In the study, four different crystal sheets are given, which are rotated typically at four different angles from 0° to 60° , that is, 0° , 6° , 12° and 30° . From Fig. 7, it is inferred that the dislocation nucleation stress increases as the atom sheet direction increase. The 0° crystal sheet in this study is armchair form sheet and the 30° crystal sheet is zigzag form sheet. The dislocation

nucleation stress in the 0° crystal sheet is less than that in the 30° crystal sheet, which is also concluded by Chang *et al.*^[13] Using the present method, we can easily obtain the dislocation nucleation stress by comparing the strain-stress curves and the strain-criterion curves. Dislocation nucleation stress of any direction crystal sheet can be obtained easily. From Fig. 7, we can clearly observe the periodicity of dislocation nucleation stress. The dislocation nucleation stresses of the 0° and 30° crystal sheets are on the bottom point and peak point of the curves, respectively. The small amplitude difference means that the zigzag crystal sheet dislocation nucleation stress is slightly greater than the one of armchair crystal sheet.



Fig. 7. Dislocation nucleation stress vs the angle change from 0° to 60° .

In summary, we have combined the continuum atomic potential method and the instability criterion to study the inhomogeneous dislocation nucleation of crystal sheet structure. By investigating the Λ criterion, we present the onset of dislocation nucleation and the criterion distribution map. The results show that the dislocation nucleation stress is related to the crystal sheet orientation angle. It should be noted that this study is based on the revised Cauchy–Born rule, considering only one internal freedom.

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