**Dislocation based Plasticity in the Case of Nanoindentation**

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**Abstract**

*Understanding plasticity initiation and evolution in a nanoindentation test is a fundamental issue. In this study, a continuum model is developed to analytically predict the force-depth curve by coupling the expanding cavity model and the evolution of dislocation density. Large-scale molecular dynamics simulations are performed to evaluate the mechanical behavior of bcc Fe under nanoindentation of a spherical indenter and to verify the continuum model. The comparison between molecular dynamics simulations and model predictions shows that the initiation and evolution of dislocation networks is strongly dependent on the loading orientation, which is associated with different deformation patterns. By introducing a scaling factor to quantify the relative size of the plastic zone, it is found that the orientation-dependence of the incipient plasticity is dominated by the elastic anisotropy and the volume of plastic zone. Appling the transition state theory, we investigate the slip-twinning transition as a function of loading rate, which supports the basic hypothesis in the continuum model that the activation of shear loop requires lower energy compared with twin nucleation, although twins can nucleate temporally and annihilate into shear loops finally.*

Keywords: Nanoindentation; Dislocations; Molecular dynamics; Shear loops; Twinning.

**1. Introduction**

Understanding the size-dependent post-elastic response [[1](#_ENREF_1)] has been an essential issue due to the explosive growth in the application of sub-µm solid state devices. In the case of crystalline materials with surface-dominated geometries (such as nanopillars) [[2-5](#_ENREF_2)], the microstructural, or *intrinsic*, size dependence of the mechanical properties is usually raised from the constraints of surfaces on the movement of dislocations. The well-known Hall-Petch relation (i.e. the smaller is the grain size the stronger is the response) emerges from the vast majority of the studies [[6-8](#_ENREF_6)] focusing on the polycrystalline bulk materials, where the grain boundaries serve as obstacles to dislocation motion. Besides, a similar strengthening effect associated with decreasing the indentation size in micro- and nano-indentation tests has been widely reported [[9-12](#_ENREF_9)]. These experimental findings, thus, suggest that the intrinsic length scale of the deformation field characterizes the inelastic behaviors of materials with size at submicron and nano scales. Since the intrinsic length scale is not involved in the conventional plasticity theories, various theories of small-scale plasticity, e.g. strain gradient plasticity (SGP) [[13-23](#_ENREF_13)], were proposed to address these size effect problems. Among enormous studies dedicated to demonstrate the physical basis of the SGP, most of which are phenomenological isotropic theories [[15-18](#_ENREF_15), [24](#_ENREF_24)] while others are established with emphasis on incorporating the intrinsic length scale of dislocation networks, such as, the mechanism-based gradient plasticity [[9](#_ENREF_9), [20](#_ENREF_20)], and the dislocation density based strain gradient model [[22](#_ENREF_22)].

Nanoindentation (generally carried out in either the load/force-controlled (LC) or displacement-controlled (DC) mode) has been widely used to measure the mechanical properties at small scales, but may be even more important as a technique to capture the initiation and evolution of plasticity in small volume. In past decades, the indentation size effect has been extensively studied in literatures, among which a strain gradient theory to explain the experimentally observed size dependence of indentation hardness was proposed [[9](#_ENREF_9), [18](#_ENREF_18), [25](#_ENREF_25)]. Established on the Taylor relation of the flow stress, the widely cited Nix-Gao model [[9](#_ENREF_9)] assumes that the flow stress as a function of total density of statistically stored dislocation and geometrically necessary dislocation. However, the phenomenological theories cannot help to deepen the physical understanding of the inherent mechanisms dominating the activation of the inelastic response. That is to say, a typical nanoindentation process can be described as follows: (a) elastic stage: an indenter with given geometry is pushed into the specimen surface, during which the maximum shear stress beneath the contact interface is lower than the critical resolved shear stress at any slip systems (however, it should be noted that at very beginning, where the contact area approaches to zero, even small loading force results in very high stress); (b) elastoplastic stage: the dislocations begin to nucleate, a characteristic phenomenon is the occurrence of a “*pop-in*” event on the force-depth curve, which corresponds to a displacement burst in LC mode or force drop in DC mode. The transition from elastic to elastoplastic stage, i.e. the first *pop-in* event, thus should be understood rigorously [[26-36](#_ENREF_26)]. Several criterions [[37-43](#_ENREF_37)] have been proposed to predict the instability in terms of a local material threshold. A widely used approach is based on the hypothesis that the dislocation nucleation is initiated once the local resolved shear stress exceeds a threshold value. Li and co-workers [[40-42](#_ENREF_40)] proposed the $Λ$ criterion, which is based on stability of phonon spectrum in a deformed crystal. Their results revealed that the homogeneous nucleation of dislocations is activated location-sensitively beneath the contact surface. Miller and Rodney [[39](#_ENREF_39)] further demonstrated that it should be cautious to use these criterions due to the non-local nature of the instability. In a recent nanoindentation study of bcc Fe-3%Si specimen, Zhang and Ohmura [[44](#_ENREF_44)] found that the “*pop-in*” represents a transition from discrete dislocation nucleation to the collective, avalanche-like dislocation multiplication. Thus, to predict the incipient plasticity more precisely, the collective behavior of dislocation networks has to be considered. Following the merit of a new criterion [[45](#_ENREF_45)] based on the linear stability of field dislocation mechanics, the non-local nucleation events can be well described by the evolution of dislocation density as a function of external loading conditions. This may indicate that the SGP theories proposed for the non-local continuum can be applied to describe the nucleation event in the initial stage of plastic deformation. Established from the classical expanding cavity model (ECM) [[46](#_ENREF_46)], Gao [[11](#_ENREF_11)] developed a new model to consider the strain-hardening and indentation size effects by incorporating the stress field solution of the phenomenological Aifantis SGP theory [[23](#_ENREF_23)]. Associated with proper yielding criterion, the Gao’s model [[11](#_ENREF_11)] could be applied to describe the non-local nucleation and subsequent multiplication of dislocations.

However, the phenomenological explanations mentioned above are established regardless of the major deformation mechanisms, i.e. the ordinary dislocation-slip plasticity and deformation twinning. Exhaustive studies have demonstrated that the slip-twinning transition is critical to control the strength of materials. In one of the earliest molecular dynamics (MD) simulations for nanoindentation, Zimmerman et al. [[47](#_ENREF_47)] found that the direction of slip rarely corresponds to the direction of the maximum resolved shear stress. Alcala et al. [[48](#_ENREF_48)] found that under nanoindentation the plasticity initiation in bcc Ta is triggered by thermal and loading-rate dependent nucleation of planar defects such as twins and unique {011} stacking fault ribbons. Large-scale MD simulations performed by Remington et al. [[49](#_ENREF_49)] also showed that the plastic deformation starts with twins, and transforms into shear loops, which then transforms into prismatic loops. Considering the plastic deformation by slip and twinning as competitive mechanisms, a constitutive approach [[50](#_ENREF_50)] has been developed to predict the slip-twinning transition for a variety of metals [[51-55](#_ENREF_51)]. These studies thereby suggest that the competition between different deformation patterns should also be considered in describing the evolution of dislocation networks.

In this paper, we proposed a continuum model to predict the evolution of applied force by considering the multiplication and annihilation of dislocation networks around the indenter/specimen contact surface. Then we conducted MD simulations of Fe, a model body-centered cubic metal, to verify the model predictions. Due to the fact that the dislocation nucleation is a stress-assisted thermo-activated process, the slip-twin competition mechanism was investigated under the framework of transition state theory (TST), which has been commonly used to predict the nucleation of dislocations [[56-61](#_ENREF_56)]. The remainder of this paper is organized as follows: in Section 2, we describe the detailed settings of MD simulations, and formulate the theoretical framework; in Section 3, model predictions and MD results are summarized and compared to the TST calculations; in Section 4, we conclude the significance of this paper.

**2. Computational details**

***2.1. MD settings***

The large-scale atomic/molecular massively parallel simulator (LAMMPS) [[62](#_ENREF_62)] is employed to perform atomistic simulations in this paper. The particle interaction between Fe atoms is described by a widely-used Finnis-Sinclair type embedded atom method potential [[63](#_ENREF_63)]. As shown in **Fig. 1**, indentation is carried out using a rigid spherical indenter tip [[43](#_ENREF_43)], which is pressed into the bulk material with three different orientations listed in **Table 1**. The periodic boundary condition is applied along the x- and y- axis in Cartesian coordinate. The time step for velocity-Verlet integration is set as 1 fs. Before applying indentation loading, the system is relaxed in a NPT ensemble for 50 ps, carried out at 300 K and 0 bar (only applied along x- and y- directions) with the Nosé-Hoover thermostat and barostat. Then, the indentation loading is applied along z-axis by penetrating a spherical indenter into the specimen up-surface with a fixed velocity. The defects detection is conducted by using the dislocation extraction algorithm (DXA) [[64](#_ENREF_64)], which transforms the original atomistic representation of a dislocated crystal into a line-based representation of the dislocation networks, thus can determine the Burgers vector of each dislocation segment and identify dislocation junctions. During the modelling, we calculate the common neighbor analysis (CNA) [[65](#_ENREF_65), [66](#_ENREF_66)] and centro-symmetry parameters [[43](#_ENREF_43)] for post-processing. The defective structures are visualized in OVITO [[67](#_ENREF_67)].

**Table 1**. Geometry of Fe specimens used in nanoindentation tests.

|  |  |
| --- | --- |
| Specimensseries | Cartesian coordinate |
| x-axis | y-axis | z-axis |
| Geo1 | [100] | [010] | [001] |
| Geo2 | [1$\overbar{1}$1] | [1$\overbar{1}\overbar{2}$] | [110] |
| Geo3 | [11$\overbar{2}$] | [$\overbar{1}$10] | [111] |

***2.2. Continuum model***

Inspired by the plasticity model developed by Krasnikov and Mayer [[68](#_ENREF_68)], here we report a dislocation-density based analytical model which is already utilized to describe the indentation response under hydrogen environment [[69](#_ENREF_69)] by considering the nucleation and subsequent multiplication of dislocations during indentation process. In nanoindentation tests [[70](#_ENREF_70)], the dislocation microstructure is generated beneath the indenter to accommodate the strain as well as the strain gradients associated with the geometry of the contact surface. Thereby, according to the SGP solution of the expanding cavity model [[11](#_ENREF_11), [71](#_ENREF_71)] of nanoindentation, the principal stresses within the interior of specimen beneath the spherical indenter can be written as,

 $σ\_{rr}=-\frac{2σ\_{Y}}{3}\left(1-\frac{r\_{c}^{3}}{r\_{o}^{3}}\right)+2\left[\frac{κ}{3n}\left(\frac{σ\_{Y}}{E}\right)^{n}\left(1-\frac{r\_{c}^{3n}}{r^{3n}}\right)-\frac{6Cσ\_{Y}}{5E}\frac{r\_{c}^{3}}{a^{5}}\left(\frac{a^{5}}{r\_{c}^{5}}-\frac{a^{5}}{r^{5}}\right)\right]$ (2.1-a)

 $σ\_{θθ}=-\frac{2σ\_{Y}}{3}\left(1-\frac{r\_{c}^{3}}{r\_{o}^{3}}\right)+2\left[\frac{κ}{3n}\left(\frac{σ\_{Y}}{E}\right)^{n}\left(1+\left(\frac{3n}{2}-1\right)\frac{r\_{c}^{3n}}{r^{3n}}\right)-\frac{6Cσ\_{Y}}{5E}\frac{r\_{c}^{3}}{a^{5}}\left(\frac{a^{5}}{r\_{c}^{5}}+\frac{3}{2}\frac{a^{5}}{r^{5}}\right)\right]$ (2.1-b)

where $r$ and $θ$ denote the coordinates in the spherical coordinate system (which can be found in the Fig. 1 of [[72](#_ENREF_72)]), $σ\_{Y}$ is the yield strength, $E$ is the Young’s modulus of the specimen, $κ,n,C$ are the constitutive parameters of the elastic-plastic material (with $κ,n,C$ are strength coefficient, strain hardening parameter and strain gradient coefficient, respectively), $a$ is the contact radius, i.e. the inner radius of the plastic region, and $r\_{c}$ is the outer radius. Assuming $F$ is the force applied on the specimen, the contact radius can be determined by the classical Hertzian elasticity [[49](#_ENREF_49)],

 $a=\left[\frac{3}{8}\frac{\left(1-υ^{2}\right)}{E}2RF\right]^{1/3}$ (2.2-a)

 $\left(\frac{r\_{c}}{a}\right)^{3}=\frac{1}{4}\frac{E}{σ\_{Y}}\frac{a}{R}$ (2.2-b)

where $R$ is the radius of the spherical indenter-tip, and $υ$ is the Poisson’s ratio of the specimen. It should be noted that the equivalent indentation elastic modulus $E^{\*}$ is defined as $\frac{1}{E^{\*}}=\frac{1-υ\_{t}^{2}}{E\_{t}}+\frac{1-υ\_{s}^{2}}{E\_{s}}$, where the subscript *t* and *s* represent indenter-tip and specimen, respectively. Since the Young’s modulus for a rigid indenter is infinite (i.e., $E\_{t}=\infty $), the equivalent modulus $E^{\*}$ is only dependent on the elastic properties of the specimen material (thus we ignore the subscript *s* for simplicity). With the principal stress known in **Eq. (2.1)**, the shear stress can be obtained,

 $σ\_{τ}=\frac{σ\_{rr}-σ\_{θθ}}{2}=-\frac{κ}{2}\left(\frac{σ\_{Y}}{E}\right)^{n}\left(\frac{r\_{c}}{r}\right)^{3n}+\frac{3Cσ\_{Y}}{Er\_{c}^{2}}\left(\frac{r\_{c}}{r}\right)^{5}$ (2.3)

If we make $\overbar{r}=r/r\_{c}$ and $\overbar{σ}\_{Y}=σ\_{Y}/E$, the equation above can be rescaled as,

 $σ\_{τ}=-\frac{κ}{2}\left(\overbar{σ}\_{Y}\right)^{n}\left(\frac{1}{\overbar{r}}\right)^{3n}+\frac{3C\overbar{σ}\_{Y}}{r\_{c}^{2}}\left(\frac{1}{\overbar{r}}\right)^{5}$ (2.4)

at the contact surface (i.e. $\overbar{r}=a/r\_{c}$), the shear stress will achieve its maximum $σ\_{τ}^{max}$. In other words, here we simply assume that the dislocation nucleation is triggered in the vicinity of the contact surface, which is also observed in the subsequent MD simulations.

As a natural derivation of the elasto-plastic response, the total indentation depth can be considered as the sum of the elastic displacement $h\_{e}$ and plastic displacement $h\_{p}$. For an incremental indentation depth $dh$, by taking the first-order derivative of it with respect to time $t$, we have,

 $\frac{dh}{dt}=\dot{h}\_{e}+\dot{h}\_{p}=v\_{i}$ (2.5)

where $v\_{i}$ is the indenter velocity. According to the Hertzian theory, the elastic displacement $h\_{e}$ is a function of the applied force $F$,

 $h\_{e}=\left(\frac{3F}{4E^{\*}\sqrt{R}}\right)^{2/3}$ (2.6)

where the $E^{\*}$ represents the equivalent elastic modulus, which has been described above. The plastic component can be written as,

 $\dot{h}\_{p}=\left(r\_{c}-a\right)\dot{w}$ (2.7)

Thus, we can obtain the ordinary differential equation (ODE) for the force evolution as follows,

 $\frac{dF}{dt}=\frac{3}{2}F^{1/3}\left[v\_{i}-\left(r\_{c}-a\right)\dot{w}\right]/\left(\frac{3}{4E^{\*}\sqrt{R}}\right)^{2/3}$ (2.8)

The characteristic deformation rate $\dot{w}$ can be described by the well-known Orowan equation,

 $\dot{w}=\frac{b}{\sqrt{6}}V\_{D}ρ\_{D}$ (2.9)

where $b$ is the module of Burgers vector, $V\_{D}$ is the dislocation velocity, and $ρ\_{D}$ is the scalar density of dislocations. The coefficient $\sqrt{6}$ originates from the projections of Burgers vectors and normal to the slip plane with certain lattice orientation onto the loading direction [[73](#_ENREF_73), [74](#_ENREF_74)]. Specifically, the dislocations are characterized by the slip plane defined by the normal vector $\vec{n}$, and by the Burgers vector $\vec{b}$ laying in this slip plane. Plastic distortion change provide by dislocation movement is given by $\dot{w}=bnV\_{D}ρ\_{D}$. In the simulations of this manuscript, the dislocation activity is mainly observed on {112} family, thus the magnitude of the normal vector is *n* = 1/$\sqrt{6}$. The dislocation velocity can be derived using the following equation of motion [[68](#_ENREF_68)],

 $βV\_{D}=b\left[σ\_{τ}^{max}-σ\_{Y}/2\right]∙\left[1-\left(V\_{D}/c\_{t}\right)^{2}\right]^{3/2}$ (2.10)

where $β$ is the phonon frition coefficient increasing with temperature [[75](#_ENREF_75)], $c\_{t}$ is the transverse sound velocity. By considering the so-called “quasi-relativistic” effect, which describes the growth of dislocation self-energy at $V\_{D}\rightarrow c\_{t}$, the **Eq.(2.10)** represents the balance of forces applied on dislocation, i.e., the phonon drag force is equal to the force caused by external stress field excluding the static yield strength $σ\_{Y}$. The left side of this equation represents the energy dissipation due to the excitation of phonons, while the drag force originating from electron scattering is negligible at the room temperature [[76](#_ENREF_76)]. In the simulations of nanovoided metals [[68](#_ENREF_68)], the neglect of the “quasi-relativistic” factor leads to the overestimation of dislocation velocity and too fast growth of voids. Because the present model is in analogy with the nanovoid model, this “quasi-relativistic” effect should also be considered. It should also be noted that the stress should remain on the yield surface if only there is enough time for the plastic relaxation realized through the dislocation motion. It takes place at very low, quasi-static, strain rates. Therefore, the used yield strength here is the static one. In dynamics, the possible rate of plastic deformation is not enough for the instantaneous relaxation of extra stresses that result in the increase of the acting shear stress with the strain rate [[77](#_ENREF_77)]. Within the framework of empirical plasticity models, it can be taken into account by the introduction of “dynamic” yield strength depending on the strain rate and other parameters. Within the present model, this effect is accounted by the final velocity and density of dislocations; therefore, we do not need to introduce the dynamic yield strength and hold the stresses on the corresponding surface. Vice versa, the resulting shear stress forms the “dynamic” yield surface. In the study of the growth of a nanovoid, Krasnikov and Mayer [[68](#_ENREF_68)] demonstrated that the homogeneous nucleation of dislocations should be considered due to the fact that the pre-existing dislocations are not enough to support the formation of effective plastic flow around the smaller void at higher strain rate. Similarly, the homogeneous dislocation nucleation is also widely applied to interpret the incipient plasticity observed in numerous nanoindentation tests [[38](#_ENREF_38), [42](#_ENREF_42), [43](#_ENREF_43), [78](#_ENREF_78), [79](#_ENREF_79)]. On the other hand, some studies [[34](#_ENREF_34), [80](#_ENREF_80)] suggested that the heterogeneous dislocation nucleation is also anticipated to better understand the effect of size scale on the process of the incipient plastcity. According to Krasnikov and Mayer [[68](#_ENREF_68)], the dislocation nucleation can be described by a typical thermally activated process equation for the probability of critical thermal fluctuation from the classical nucleation theory. Well established in statistical physics, the total energy of each atom in a thermodynamic ensemble can be described by the Boltzmann distribution, in which the ratio of the total energy and thermal fluctuation defines the logarithmic fraction of the atoms with a given energy. The nucleation of dislocations in a fluctuation manner thus occurs if the energy of thermal motion of some atoms exceeds the energy barrier required for the rearrangement of atoms to a metastable position, with details described in [[68](#_ENREF_68)]. Associated with the energetic picture, the dislocation density evolution thus can be divided into the contributions of homogeneous and heterogeneous multiplication and net annihilation,

 $\frac{dρ\_{D}}{dt}=\left(\frac{dρ\_{D}}{dt}\right)\_{hom}+\left(\frac{dρ\_{D}}{dt}\right)\_{het}-\left(\frac{dρ\_{D}}{dt}\right)\_{ann}$ (2.11)

where the first term in the right side represents the homogeneous nucleation of dislocations,

 $\left(\frac{dρ\_{D}}{dt}\right)\_{hom}=ξ∙L∙N∙N\_{1}∙Π=\frac{πc\_{t}}{2V\_{s}}\left(\frac{2πb\left(r\_{c}^{2}-a^{2}\right)}{a\_{cr}^{3}}\right)exp\left(-\frac{ΔE\_{c}}{k\_{B}T}\right)$ (2.12)

where $ξ=c\_{t}/2a\_{cr}$ is the (attempt) characteristic frequency for dislocation emission with $a\_{cr}$ as the critical radius of the emitted semi-circular dislocation loop, $L=2πa\_{cr}$ is the length of the emitted dislocation loop, $N=1/V\_{s}$ (where $V\_{s}$ is the volume of the specimen, equals to $d^{2}t\_{h}$ ($t\_{h}$ is the thickness defined in **Fig. 1**)) is the number of areas close to the contact surface where the dislocation nucleation occurs, and the number of nucleus in the plastic zone can be estimated as $N\_{1}=2πb\left(r\_{c}^{2}-a^{2}\right)/a\_{cr}^{3}$ according to the original definition in Ref [[68](#_ENREF_68)]. However, the characteristic size of the plastic is actually controlled by the yield strength (see **Eq. (2.2-b)**), which is strongly dependent on the specimen size [[81](#_ENREF_81)]. Besides, since the derivation of **Eq. (2.2-b)** is made of Taylor’s expansion with all non-linear terms truncated, Gao et al. [[82](#_ENREF_82)] pointed out that this approximation works well for spherical indenter with small *a*/*R*. Considering the larger ration between the indenter radius and specimen size used in the following simulations, we re-estimate the plastic zone volume with the empirical formula proposed by Durst et al. [[83](#_ENREF_83)] as $V\_{p}=\frac{2}{3}π[(fa)^{3}-a^{3}]$, where the scaling factor is 1<= *f* <=3.5 for the process with a Berkovich indenter in fcc Cu. This scaling factor is merely an empirical parameter depending on the strain limit defining the boundary between the elastic and plastic zones, thus does not have to be limited in the range of [1, 3.5] in present scenario with a spherical indenter penetrating into bcc Fe specimens. This is a major improvement to consider the indentation size effect, compared with our previous model [[69](#_ENREF_69)], which is designed to describe the effect of (hydrogen) interstitials on the incipient plasticity. Thus, the number of nucleus can be rewritten as $N\_{1}=V\_{p}/a\_{cr}^{3}$. The probability of thermal fluctuation leading to the dislocation nucleation is estimated as [[68](#_ENREF_68)],

 $Π=exp\left(-\frac{ΔE\_{c}}{k\_{B}T}\right)=exp⁡\left(-\frac{πϵ\_{s}^{2}}{2bσ\_{τ}^{max}k\_{B}T}\right)$ (2.13)

where $ϵ\_{s}$ is the formation energy of dislocation per unit length, which typically ranges from ~ 0.2 to 0.4 eV/*b* [[84](#_ENREF_84)], and $k\_{B}$ is the Boltzmann constant. And the second term, which represents the heterogeneous nucleation of dislocations, can be described by connecting the energy irreversible spending on the plastic deformation and the energy of dislocation formation in continuum mater,

 $\left(\frac{dρ\_{D}}{dt}\right)\_{het}=\frac{0.1}{ϵ\_{D}}\left(b∙σ\_{τ}^{max}∙V\_{D}\right)ρ\_{D}$ (2.14)

where $ϵ\_{D}$ is the line energy of dislocation per unit length [[85](#_ENREF_85), [86](#_ENREF_86)]. The third term in the right side of **Eq.(2.12)** comes from the annihilation of dislocations with opposite Burgers vector, reads as [[87](#_ENREF_87), [88](#_ENREF_88)],

 $\left(\frac{dρ\_{D}}{dt}\right)\_{ann}=k\_{a}bV\_{D}ρ\_{D}^{2}$ (2.15)

where $k\_{a}$ is the annihilation factor, which is increasing with temperature rise [[88](#_ENREF_88)]. Thus, the total rate of dislocation production becomes,

 $\frac{dρ\_{D}}{dt}=\frac{πc\_{t}}{2V\_{s}}\left(\frac{2π\left(f^{3}-1\right)a^{3}}{3a\_{cr}^{3}}\right)exp\left(-\frac{ΔE\_{c}}{k\_{B}T}\right)+\frac{0.1}{ϵ\_{D}}\left(b∙σ\_{τ}^{max}∙V\_{D}\right)ρ\_{D}-k\_{a}bV\_{D}ρ\_{D}^{2}$ (2.16)

Now the ODE **Eq.s-(2.8)&(2.16)** can be solved in a MATLAB utility with the fourth order Runge-Kutta technique. The introduction of hardening parameters will allow us to compare the nanoscale experiments and simulations directly with finite element method simulations. Here we consider the indentation of initially perfect single crystal without the presence of dislocations, i.e. the nucleation is the only mechanism providing the incipient dislocation density. It should be noted that the initial dislocation density could be taken into account in both Krasnikov-Mayer model and the present model if one let the initial value of $ρ\_{D}$ to be non-zero. As mentioned in [[68](#_ENREF_68)], the model predictions are compared with the MD results for samples initially containing the lattice defects, where the presence of initial dislocation can suppress the nucleation and provide multiplication as the only source of new dislocations, but the specific scenario depends on the strain rate and initial state of the sample (i.e. the various combinations of materials parameters). In **Fig. 2**, we plot the predicted force-depth curves with different initial dislocation densities. The loading condition is set as, *d* = 80 nm, *t* = 80 nm, *R/d* = 0.1 and $v\_{i}$ = 0.5 Å/ps, and the materials parameters are chose as $E\_{110}=219.3$ GPa and *f* = 1.5. All the necessary parameters are listed in **Table 2**. The maximum value of the force-depth curve is defined as the “*pop-in*” force. As shown in **Fig. 2**, the “*pop-in*” force will decease with the initial dislocation density monotonically. By accurately choosing physical parameters and comparing to nanoindentation experiments, this model can be used to calibrate the materials parameters used in macro-scale simulations. However, it should be noted that once the initial dislocation density is not equal to zero, the determination of material parameters, e.g. the $k\_{a}$, $ϵ\_{s}$ and $ϵ\_{D}$, will become much more sophisticated.

**Table 2**. Parameters of Fe matrix used in current model.

|  |  |
| --- | --- |
| Parameters | Value |
| Burgers vector $b$ [[76](#_ENREF_76)] | 0.229 nm |
| Dislocation annihilation factor $k\_{a}$ [[88](#_ENREF_88)] | 0.5 |
| Dislocation formation energy $ϵ\_{s}$ [[68](#_ENREF_68)] | 0.136 eV |
| Dislocation line energy $ϵ\_{D}$ [[76](#_ENREF_76)] | 8 eV/$b$ |
| Strength coefficient $κ$ | 2.65 GPa |
| Strain hardening parameter $n$ [[89](#_ENREF_89)] | 0.12 |
| Strain gradient coefficient $C$ [[90](#_ENREF_90)] | 2.5 N |
| Phonon friction coefficient $β$ [[75](#_ENREF_75)] | 2.5\*10-14 GPa\*s |
| Poisson’s ratio $v$† | 0.29 |
| Transverse (Shear) sound velocity $c\_{t}$ | 3.24 km/s |
| Yield strength $σ\_{Y}$ [[76](#_ENREF_76)] | 0.17 GPa |
| Young’s modulus $E$†† | 131.2,219.3,282.5 GPa |

† As demonstrated by Meyers and Chawla [[91](#_ENREF_91)], in the anisotropic materials, the Poisson’s ratio depends on the orientation and for each loading direction one can have more than one value of it. Thus, for simplicity, here we use an average value for different loading scenarios in all the computations.

†† The computational details of the Young’s moduli along [100], [110], and [111] for iron can be found in the **Appendix A**.

**3. Results and discussion**

**3.1. *Analysis of the first yielding event***

Due to the fact that the characteristic length of the mean free path of dislocation networks is at the magnitude of nanometer, the mechanical response of a nanocrystal is significantly affected by the size of the specimen. In order to map out the size effect on the indentation response, we designed a series of simulations for the Fe specimens with different width *d*. The indenter velocity is fixed at 0.5 Å/ps. The size along z-axis for all specimens is fixed at 80 nm to ensure that the surface interaction would be eliminated. The ratio of indenter radius *R* and width *d* is fixed at *R*/*d* = 0.225. The obtained force-depth curves are shown in **Appendix B**. The force-drop phenomenon can be clearly observed in all the indentation experiments of Geo1 specimens compared with the other two geometries. In **Fig. 3**-(a-c), the critical force, which marks the incipient “*pop-in*” behavior on the force-depth curves, is plotted as a function of the specimen size together with the predictions of the continuum model for three different loading orientations, respectively. For the absolute value of the critical force, it follows the order: [001] > [111] > [110], and agrees with the MD simulations of bcc Ta performed by Remington et al. [[49](#_ENREF_49)]. Using a *R*/*d* = 0.267, Alcala et al. [[48](#_ENREF_48)] also studied the orientation dependency of Ta under nanoindentation, and obtained the result as: [001] > [110] > [111]. The difference could be caused by the other simulation parameters, such as indenter radius, penetration rate and specimen thickness. Dependent on the indenter radius, Shim et al. [[92](#_ENREF_92)] found a clear reduction of the *pop-in* load for crystals with increasing pre-deformation, indicating a change in the nucleation mechanism from homogeneous to heterogeneous. [[31](#_ENREF_31)] have demonstrated that the hardening exponent strongly depends on the variation of the indenter tip radius and indentation depth. Li et al. [[93](#_ENREF_93)] attributed the orientation dependence of the *pop-in* loads to the anisotropy of indentation Schmid factor in the experimental study of NiAl single crystals. The nanoindentation tests of single crystal copper [[94](#_ENREF_94)] also show that the indentation pile-up patterns under spherical indenter exhibit four-, three- and two-fold symmetries for the [100], [111] and [011] orientations, respectively. By incrementally changing the scaling factor *f*, we found that the relative “thickness” of the plastic zone deceases with increasing specimen size. It is intuitive to understand this phenomenon in a kinetic way, i.e. the activation of the incipient plasticity requires a critical volume of the plastic zone. Thus, with increasing specimen size *d*, due to the fixed ratio of *R*/*d*, the indenter radius would increase and consequently lead to the enlargement of the surface area of the plastic zone. Therefore, for a given activation volume, the required “thickness” of the plastic zone would decrease. Detailed analysis of dislocation behavior in **Section 3.2** shows that this orientation dependence is related to the activated dislocation configurations at the incipient plasticity. We noticed that in the indentation tests of Geo1 specimens, the plasticity is initiated before the first obvious *pop-in* [[95](#_ENREF_95)], which suggests that dislocations are not homogeneously nucleated within the plastic zone in experiments [[96](#_ENREF_96)]. In **Fig. 4**-(a), we can observe the nucleation of the flattened octahedral structure (FOS) which has been reported in the atomistic simulations of compression [[97](#_ENREF_97)] and tension tests [[56](#_ENREF_56), [98](#_ENREF_98)], and can serve as the precursor of dislocation nucleation. As demonstrated by Pang et al. [[98](#_ENREF_98)], the dislocation is generated via a three-stage procedure, in which random FOSs are activated by thermal fluctuations, then form double-layer defect clusters, which finally evolve into dislocations due to relative slip of internal atoms.

With all the specimens having a fixed width (80 nm) and thickness (80 nm), we studied the radius effect and found that the indentation force is expected to increase with increasing radius of indenter tip. In **Fig. 3**-(d-f), the critical force as a function of the normalized radius is plotted. It is found that the critical force still follows the order: [001] > [111] > [110]. Compared with the model predictions, it is still found that the scaling factor *f* deceases with increasing indenter radius. While for a fixed scaling factor *f*, the continuum model predicts that the critical “*pop-in*” force decreases with the normalized radius. Nix and Gao [[9](#_ENREF_9)] have pointed out that the strengthening effect arising from strain gradient plasticity has to be considered. Reflected in the present model, it is the size of the plastic zone dominating the elasto-plastic response beneath the indenter. A simplified model based on the strain gradient plasticity developed by Lee et al. [[12](#_ENREF_12)], which agrees with the experimental data well, also demonstrates that the “characteristic length” quantifying the size of the plastic zone dominates the elasto-plastic behavior during the indentation process.

Due to the fact that the free surface is introduced by applying non-periodical condition along z-axis, the thickness effect is studied in **Fig. 3**-(g). The width *d* = 80 nm, indenter tip radius *R* = 0.225*d*, and the loading velocity $v\_{i}$ = 0.5 Å/ps. It is found in all the simulations shown in **Fig. 3**-(g), the critical force follows the order: [001] > [111] > [110]. Compared with other geometry parameters, it seems that the “*pop-in*” behavior is not sensitive to the change of thickness. This result is reasonable because the thickness is large enough to assure that the plastic zone is not affected by the free surface along z-direction. However, the weak dependence between the “pop-in” force and the specimen thickness shown in MD simulations, does not mean that the size of plastic zone is independent with the specimen thickness. Compared with the model predictions (shown as the dash lines), it is found that the scaling factor *f* slightly increases with the specimen thickness. In this figure, we can also clearly found that the scaling factor *f* follows the order: [001] < [111] < [110], although the difference of the *f* between [111] and [110] scenarios is indeed very small. This result thus demonstrates that the incipient plasticity can be easily activated in the specimens loaded along the [100] direction. The dislocation analysis shown in the following section supports this conclusion by the evidence that the FOSs would be pre-nucleated before the nucleation of dislocation loops. Nair et al. [[80](#_ENREF_80)] performed atomistic studies about the effects of thickness on the mechanical response in the Ni single crystals under nanoindentation. They found that the critical force decreases with the increase of the specimen thickness. However, they used an indenter with the tip radius of 30 nm, which is much larger than the thickness 12.8 nm. Thus, the plastic zone would be strongly affected by the free surface in their simulations.

In order to gain more insights about incipient plasticity, we derive the stress-strain curve under uniaxial compression associated with nanoindentation by Tabor’s relation [[72](#_ENREF_72), [99](#_ENREF_99)], which reads as,

 $σ=\frac{p\_{m}}{ψ}=\frac{F/A}{ψ}$ (3.1)

 $ε=0.2\frac{a}{R}$ (3.2)

where $σ$ and $ε$ are the flow stress and strain in uniaxial compression, $p\_{m}$ is the mean indentation pressure, $ψ$ is the plastic constraint factor (taken as 3 [[72](#_ENREF_72), [99](#_ENREF_99)]), and $A$ is the cross-sectional contact area of the indenter. Here the coefficient 0.2 is actually an empirical parameter defined by Tabor [[100](#_ENREF_100)], who found that the mean indentation pressure $p\_{m}$ scaled by the plastic strain factor $ψ$ when plotted against $0.2a/R$ matches excellently with the simple compression stress-strain curves. As shown in **Fig. 3**-(h), the maximum stress of the specimen loaded at [001] direction is ~ 6.4 GPa, which is larger than that of other two loading directions. This is due to the fact that the plasticity is initiated by the nucleation of FOSs in the [001] loaded specimen. It is also found that for all three loading directions the stress will saturate to a similar level after plastic yielding. Besides, the elastic response is almost independent on the loading direction, which suggests that only the nucleation event is significantly affected by the loading conditions. The great discrepancy of [001] yielding behavior from the other two specimens also indicates that the detailed deformation patterns are different, which will be confirmed by direct observation of defect structures in next section. According to $τ\_{max}=\left(1-2ν\right)σ/2\left(1-ν\right)$, the global maximum shear stress $τ\_{max}$ data from experiments [[26](#_ENREF_26)] can be related with the uniaxial tension stress $σ$, which is in the range of 3.80±0.15 GPa for (111), 3.67±0.15 GPa for (101) and 3.16±0.42 GPa for (001) orientation, respectively. The agreement between experimental data and present MD simulations further demonstrates the orientation dependence of mechanical response during nanoindentation process.

**3.2. *Evolution of dislocation networks***

The MD results of the critical forces in **Fig. 3** show that the plastic deformation of bcc Fe is strongly dependent on the loading direction. To understand the underlying mechanisms, we present the snapshots obtained from MD simulations in this section. The specimens (~ 31 million atoms) have the same simulation settings, which are *d* = 90 nm, *t* = 45 nm, $v\_{i}=$ 20 m/s, and *R*/*d* = 0.1. We have also performed the simulations under $v\_{i}=$ 4 m/s, which does not affect the plastic behavior significantly.

**I. *Loading along [001] direction***

In **Fig. 4**-(a), it can be observed that FOSs are activated underneath the indented surface. With continuous loading, the FOSs condense into 4 clusters. Shear loops are then nucleated in these FOS clusters, but not from the indenter/specimen contact surface. However, in experiments, one has to consider the surface roughness [[47](#_ENREF_47)] which is not included in present paper. In **Fig. 4**-(b), we observe that shear loops form and propagate along $\left〈111\right〉$ directions. MD simulations performed by Kumar et al. [[101](#_ENREF_101)] show that the {110} and {123} slip families dominate the dislocation behaviors in bcc Fe under nanoindentation, while the {112} family is less active. As depicted by Remington et al. [[49](#_ENREF_49)], these shear loops move by the transmission of edge components and limited cross-slip of screw components, which leads to the formation of prismatic loops by pinching off the front of shear loops. The snapshots about the evolution of dislocation networks shown here are different from the results for bcc Ta [[48](#_ENREF_48)], where the incipient defect structure is an array of (011) stacking faults. This difference may be due to that the stacking fault energy of Ta is smaller than that of Fe [[102](#_ENREF_102)]. In **Fig. 4**-(c)&(d), prismatic loops are generated along four $\left〈111\right〉$ directions. Similar process was also observed by Ruestes et al. [[103](#_ENREF_103)] in the study of bcc Ta.

**II. *Loading along [110] direction***

For the tests loaded long [110] direction, it is found that the first dislocation 1/2[$\overbar{1}\overbar{1}$1] is nucleated from the contact surface at *h* = 8 Å in **Fig. 5**-(a). What we found here is consistent with the conclusions of [[48](#_ENREF_48), [49](#_ENREF_49)], i.e. the plasticity starts with the nucleation of twin boundaries, which will annihilate into shear loops subsequently. Then, complex dislocation network is developed and a prismatic loop is formed along [$\overbar{1}\overbar{1}$1] direction, shown in **Fig. 5**-(b)&(c). In **Fig. 5**-(d), another prismatic loop is generated along [$\overbar{1}\overbar{1}\overbar{1}$] direction. We can find that this 1/2[$\overbar{1}\overbar{1}\overbar{1}$] loop is formed by the pinching-off mechanism proposed by Remington et al. [[49](#_ENREF_49)]. The detailed procedure is that in **Fig. 5**-(c), the screw components marked by red arrows are with opposite signs and cancel with each other through a “lasso” action. The prismatic loops in **Fig. 5** have approximately triangular shape, which is consistent with the results of nanovoided Ta [[54](#_ENREF_54)].

**III. *Loading along [111] direction***

For the tests loaded along [111] direction, we can find that the incipient plasticity starts with the accumulation of FOSs and the successive formation of planar defects in **Fig. 6**-(a). With continuous penetration, the {112} twins nucleate, as shown in **Fig. 6**-(b). And this observation is consistent with the results of [[48](#_ENREF_48)]. In **Fig. 6**-(c), shear loops are generated due to the annihilation of multiple twins. In **Fig. 6**-(d). During the evolution, the loops do not detach from the contact surface. This will lead to the generation of steps on the contact surface.

In general, the observed dislocation behaviors demonstrate why the *pop-in* load for the specimens loaded along [110] and [111] directions are lower than that of the specimen loaded along [001] direction, where the homogeneous nucleation of dislocation loops in the deformed specimen is activated with the specific FOSs already formed. While in the [110] and [111] specimens, the heterogeneous nucleation of planar defects from contact surface is observed as the incipient plasticity. Consistent with the **Fig. 3**-(h), the yielding of [001] specimen requires a larger stress than that of the other two specimens. These observations may suggest that the proposed model should be modified by considering the orientation dependent competition between homogeneous and heterogeneous nucleation mechanisms. Besides, the dislocation nucleation from the contact surface shown in the **Fig. 5** & **6** also demonstrates why the model predictions agree better with the MD results of [110] and [111] specimens than that of [001] specimen, because in Eq. (2.4) we have already assumed that the dislocation nucleation is initiated at the contact surface.

***3.3 Predictions of the deformation patterns***

The difference in the mechanical responses of the specimens with different lattice orientations is thereby attributed to the variance of plastic deformation patterns, i.e. the competition between dislocation loops and twins. As demonstrated by Remington et al. [[49](#_ENREF_49)], the slip-twin transition has to be considered when the specimen is loaded at high strain rate. In a previous study of the strain rate effect on the plasticity initiation in nanovoided metals [[56](#_ENREF_56)], we introduced the nudged elastic band method to evolve the rate dependence. In [[93](#_ENREF_93)], the authors reviewed three different models for homogeneous dislocation nucleation (i.e. the Volterra dislocation analysis, the Peierls model and MD simulations), and found that the activation energy can be fitted to an equation of Arrhenius type. Here we present a similar analysis by mapping the minimum energy path of this Arrhenius type transition process, although in practical experiments the contribution of heterogeneous nucleation cannot be neglected [[93](#_ENREF_93)]. According to the assumptions made in [[49](#_ENREF_49)], two alternative scenarios are considered here: the nucleation of a shear loop of 1/2$\left〈111\right〉$ dislocation and the nucleation of a three-layered twin with three 1/6$\left〈111\right〉$ loops. This consideration is also consistent with the DXA analysis of our MD results shown in **Figs. 4**-**6**. The change of total energy during the formation of a shear loop reads as the sum of the elastic energy and the work done by the shear stress,

 $∆E\_{s}=\frac{r\_{s}Gb\_{s}^{2}}{4}\left(1+\frac{1}{1-υ}\right)ln\frac{2r\_{s}}{φb\_{s}}-τb\_{s}πr\_{s}^{2}$ (3.3)

where $r\_{s}$ is the radius of the shear loop, $φb\_{s}$ is the core radius, and $τ$ is the shear stress. Taking the first-order derivative of the total energy and making it equal to zero gives the critical radius of shear loop,

 $r\_{sc}=\frac{Gb\_{s}}{8πτ}\left(\frac{2-υ}{1-υ}\right)\left[ln\left(\frac{2r\_{sc}}{φb\_{s}}\right)+1\right]$ (3.4)

Thus the energy of critical shear loop nucleus is,

 $ΔE\_{sc}=b\_{s}r\_{sc}\left[πτr\_{sc}-\frac{Gb\_{s}}{4}\left(\frac{2-υ}{1-υ}\right)\right]$ (3.5)

Repeating the procedure for a twin, we have to add a term to account for the two twin boundaries formed, with energy per unit area equal to $γ\_{T}$,

 $ΔE\_{T}=\frac{3r\_{T}Gb\_{T}^{2}}{4}\left(\frac{2-υ}{1-υ}\right)ln\frac{2r\_{T}}{φb\_{T}}+2πr\_{T}^{2}γ\_{T}-3τb\_{T}πr\_{T}^{2}$ (3.6)

where $b\_{T}$ is the burgers vector of the twin partial dislocation, and $γ\_{T}$ is the twin-boundary energy. The value ‘*3*’ appearing in the first and third term in the right side means it is a three-layered twin. Through the application of **Eq.-(3.4)** it leads to,

 $r\_{Tc}=\frac{3Gb\_{T}^{2}}{8π\left(3τb\_{T}-2γ\_{T}\right)}\left(\frac{2-υ}{1-υ}\right)\left[ln\left(\frac{2r\_{Tc}}{φb\_{T}}\right)+1\right]$ (3.7)

Thus the energy of critical twin nucleus is,

 $ΔE\_{Tc}=r\_{Tc}\left[π\left(3τb\_{T}-2γ\_{T}\right)r\_{Tc}-\frac{3Gb\_{T}^{2}}{4}\left(\frac{2-υ}{1-υ}\right)\right]$ (3.8)

The critical loop radius is calculated by means of Newton iteration implemented in a MATLAB utility. Then, we can obtain the activation energy required for the critical nucleation event, given by **Eq.s-(3.6)&(3.8)**. The twin boundary energy, $γ\_{T}$ = 0.26 J/m2, is taken from [[104](#_ENREF_104)]. Gao et al. [[105](#_ENREF_105)] obtained the result of 0.3 J/m2 by means of MD simulations. The other parameters used in numerical calculations are: *G* = 82 GPa, $b\_{s}$ = 0.24855 nm, $b\_{T}$ = 0.08285 nm, $υ$ = 0.29. We choose $ρ$ = 2 according to the *ab-initio* calculations [[106](#_ENREF_106)]. According to the continuum framework proposed by Weinberger et al. [[57](#_ENREF_57)], we use the following function to fit the activation energy data,

 $∆E(τ)=A\left[1-exp\left(α\left(1-\frac{τ}{τ\_{0}}\right)\right)\right]$ (3.9)

where $A$, $α$ and $τ\_{0}$ are fitting parameters. Then, considering the dislocation nucleation is a thermos-activated process, we can use the energy barriers calculated above to predict the most probable reaction path under the framework of TST. According to Zhu et al. [[61](#_ENREF_61)], under constant temperature and strain rate, the nucleation stress can be expressed implicitly as the following equation,

 $\frac{ΔE(τ,T)}{k\_{B}T}=ln\frac{k\_{B}TNv\_{0}}{E\dot{ϵ}Ω(τ,T)}$ (3.10)

where $Nv\_{0}$ represents the number of potential nucleation sites in the plastic zone (shown in **Fig. 1**) multiplied by the attempt frequency, which is estimated to be 3×1012 s-1 for fcc Cu [[61](#_ENREF_61)], and treated as the Debye frequency ($v\_{0}=k\_{B}T\_{D}/ℏ$, where the Debye temperature of Fe is 470 K) in Ref [[57](#_ENREF_57)]. As a first approximation, we can phenomenologically take $∆E\left(τ,T\right)=(1-T/T\_{m})∆E(τ)$, where $T\_{m}$ is the surface disordering temperature. The activation volume from this functional form is,

 $Ω(τ)=\frac{Aα}{τ\_{0}}exp\left(α\left(1-\frac{τ}{τ\_{0}}\right)\right)$ (3.11)

Then, the activation volume also follows the similar expression $Ω\left(τ,T\right)=(1-T/T\_{m})Ω(τ)$. To calculate the nucleation sites, we need to assess the volume of plastic zone shown in **Fig. 1**. The contact radius of the plastic zone is described in **Eq.-(2.2-a)**.According to the Nix-Gao theory [[9](#_ENREF_9)], the total loop length yielded at the critical depth is [[49](#_ENREF_49)],

 $λ=πζ\_{a}\frac{a^{2}}{b}=0.66π\frac{a^{2}}{b}$ (3.12)

The number of nucleation sites is then calculated as,

 $N=\frac{V\_{p}}{λπ\left(φb\right)^{2}}=\frac{2(f^{3}-1)a}{3ζ\_{a}πφ^{2}b}=\frac{(f^{3}-1)a}{0.99πφ^{2}b}$ (3.13)

In order to clearly show how the nucleation stress is evaluated, we draw the solving procedure in **Fig. 7**. It is found that the orientation-dependent elastic parameters and the scaling factor would determine the final result of the nucleation stress if we assume other physical quantities, e.g. the surface disordering temperature and the dislocation radius etc., are the same for both the dislocation loop and twin nucleation scenarios. In **Fig. 8**, we plot the nucleation stress as a function of strain rate. Considering the complicated anisotropy of the shear deformation, without loss of generality, here we demonstrated two scenarios, i.e. the shear on the {100} plane (marked as “*shear*1”) and the one along the [111] on the {110} plane (marked as “*shear*2”), with the computational details shown in **Appendix A**. It should be noted that the “*shear*1” scenario is just for demonstration, not one of the 48 slip systems for the bcc structure. The results in **Fig. 8**-(a)&(c) also show that the unreal “*shear*1” behavior requires higher nucleation stress than the one for the real “*shear*2” slip. It is found that the homogeneous nucleation of twin boundaries requires a higher stress than that of a shear loop. The TST calculation is consistent with the MD findings shows in Section 3.2, where the twin boundaries can only be nucleated from the contact surface heterogeneously. Furthermore, once the planar defects are nucleated, the local stress will be relieved and lead to the annihilation of twin boundaries. The predicted stress value is also consistent with the one derived from MD simulations in **Fig. 3**-(h). Although this prediction agrees with the DXA measurements made in **Fig. 4**-**6**, it still need to be mentioned that: (1) present calculation is performed on the hypothesis that the defect is nucleated in an infinite large matrix, while in MD simulations the geometrical constrains have to be considered; (2) the lattice defect is assumed to nucleate homogeneously in the analytical framework, but in MD simulations we found that the dislocation nucleation originates from the accumulation of FOSs, which is consistent with the results of nanovoided Fe [[56](#_ENREF_56)]. Besides, all the results presented in **Fig. 8** are calculated with one constant dislocation radius ($φ=2$), which could be also orientation-dependent. To summarize, the formation of shear loops is the dominating pattern of plastic deformation in bcc Fe under nanoindentation, although twins can nucleate heterogeneously from the contact surface and annihilate into shear loops finally.

**4. Concluding remarks**

This study investigates the elasto-plastic response of bcc Fe under the indentation loading with a spherical indenter. Considering the dislocation nucleation as an Arrhenius type event, an analytical model is proposed to describe the “*pop-in*” behavior. The main results can be concluded as follows:

1. Based on the hypothesis that plasticity is initiated both homogeneously and heterogeneously in the plastic zone beneath the contact surface, a continuum model is proposed to reproduce the force-depth evolution. The comparison of model predictions with MD simulations shows that the first yielding event in the specimens loaded along the [100] direction requires a smaller plastic zone (represented by a smaller value of the scaling factor *f*), while for the ones loaded along [110] and [111] directions, a larger plastic zone is required. This is due to the fact that the dislocation nucleation in the specimen loaded along [001] direction is activated by the homogeneous formation of FOSs in the deformed crystal, while the plasticity in the ones loaded along [110] and [111] direction starts with the nucleation of twin boundaries. Based on the SGP solution of the stress field in an expanding cavity model, the present continuum model can fairly describe the non-local feature of dislocation nucleation, observed in both the previous studies and present MD simulations.

2. The slip-twinning transition is studied under the framework of transition state theory. The results show that the shear loop is much easier to be nucleated homogeneously and maintained than twin boundaries. The TST prediction is also consistent with MD simulations, where the twin boundaries can nucleate heterogeneously, but finally will annihilate into shear loops.

The theoretical framework formulated in this paper, especially with the introduction of the scaling factor to characterize the relative size of the plastic zone, can provide a general description for the nanoindentation tests of materials with elasto-plastic response.

**Acknowledgement**

K.Z. and Z.Z. acknowledge the financial support provided by the Research Council of Norway under HIPP project (Grant No. 234130/E30). A.E.M. thanks for the support from the Ministry of Education and Science of the Russian Federation (project No. 3.2510.2017/PP). All simulations are carried out on the NOTUR (Grant No. NN9110K, NN9391K) high performance computer clusters Vilje at NTNU, Trondheim and Stallo at UiT, Tromsø.

**Appendix A**

Here we present the computational details of the anisotropic Young’s moduli of bcc Fe along three different directions. Use the Eq. (2.20) in Ref [[91](#_ENREF_91)]:

 $\frac{1}{E\_{ijk}}=S\_{11}-2\left(S\_{11}-S\_{12}-\frac{1}{2}S\_{44}\right)×\left(l\_{i1}^{2}l\_{j2}^{2}+l\_{j2}^{2}l\_{k3}^{2}+l\_{i1}^{2}l\_{k3}^{2}\right)$ (A.1)

where the direction cosines are calculated as follows:

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | $$l\_{i1}$$ | $$l\_{j2}$$ | $$l\_{k3}$$ | $$l\_{i1}^{2}l\_{j2}^{2}+l\_{j2}^{2}l\_{k3}^{2}+l\_{i1}^{2}l\_{k3}^{2}$$ |
| [100] | 1 | 0 | 0 | 0 |
| [110] | $\sqrt{2}$/2 | $\sqrt{2}$/2 | 0 | 1/4 |
| [111] | 1/$\sqrt{3}$ | 1/$\sqrt{3}$ | 1/$\sqrt{3}$ | 1/3 |

The compliances of bcc Fe are:

*S*11 = 0.762 [10-2GPa-1]

*S*44 = 0.858 [10-2GPa-1]

*S*12 = −0.279 [10-2GPa-1]

This yields:

*E*100 = 131.2 [GPa]

*E*110 = 219.3 [GPa]

*E*111 = 282.5 [GPa]

The calculation of the shear moduli is a little complicated, since it involves a direction of shear ***m*** = [uvw] and plane of shear (hkl) (thus can be determined by the planar normal vector ***n*** = [hkl]) [[107](#_ENREF_107), [108](#_ENREF_108)]:

 $\frac{1}{4G(m,n)}=\frac{1}{4}S\_{44}+\left(S\_{11}-S\_{12}-\frac{1}{2}S\_{44}\right)P(m,n)$ (A.2)

where the directional function is defined as,

 $P(m,n)=P(n,m)=\sum\_{i=1}^{3}\left(m\_{i}n\_{i}\right)^{2}$ (A.3)

For the purpose of demonstration, we just calculate the shear modulus on the {100} plane and the one along [111] on the {110} plane:

$G\_{\{100\}}=\frac{1}{S\_{44}}=116.6$ [GPa]

$G\_{\{110\}}^{[111]}=\frac{3}{S\_{44}+4\left(S\_{11}-S\_{12}\right)}=59.7$ [GPa]

**Appendix B**

The indentation force as a function of depth for different loading conditions are shown as below. It can be found that the nucleation event occurring in the (001) specimens is obviously different with that in the other two specimens. This difference indicates that the large force drop observed in the indentation tests of the (001) specimens is mainly dominated by the non-local homogeneous nucleation of dislocations, while in the (110) and (111) specimens the heterogeneous nucleation from contact surface is favored. With a fixed indenter radius, the variance of the slope at elastic stage shown in **Fig. B1** and **B2** suggests that the reduced elastic modulus $E^{\*}$ defined in Eq. (2.6) changes with the radius of the indenter tip, while the **Fig. B3** shows that the elastic modulus is not sensitive to the change of the specimen thickness. According to the Eq. (3.12) [[83](#_ENREF_83)], the size of the plastic zone is proportional to the contact radius (approximately the indentation depth when it is smaller than the indenter tip radius in present MD simulations), the **Fig. B2** demonstrates that the critical size of the plastic zone required for the incipient yielding depends almost linearly on the indenter tip radius, thus suggests a non-local feature [[39](#_ENREF_39)] of the nucleation events observed in the MD simulations.

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