Atomistic simulations of nanoindentation in single crystalline tungsten: The role of interatomic potentials

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The design of the next generation of nuclear fusion machines needs efficient Plasma Facing materials (PFMs) that can withstand extreme operating conditions due to the direct interaction with the fusion plasma, and BCC metals can fulfill these requirements, in particular tungsten. However, the understanding of the behavior of these materials at extreme operating conditions, such as irradiation and high temperatures, also depends on the capacity for efficient molecular simulations using appropriate interatomic potentials. In this work, we perform Molecular dynamics (MD) simulations to emulate experimental nanoindentation tests of crystalline pure [111] W by two different Embedded Atom Method (EAM)-based interatomic potentials for describing the interaction of W-W and W-H/W-W, respectively. The characterization of W mechanical properties is done by a detailed analysis of the dislocation nucleation and evolution during the early stages of the elastic to plastic deformation transition. Results lead to similarities between load displacements curves and pileup formation for both MD potentials. However, a discrepancy is observed in the dislocation dynamics and stacking fault formation mechanism during nanoindentation, that is attributed to the difference of lattice constants, thus the Burgers vector magnitude, being directly related to stacking fault and dislocation energies.

Keywords: Dislocations dynamics, Tungsten, nanoindentation, Hardness

I. INTRODUCTION

The development of novel technology in aerospace, electronic, medical and energy industries requires the use of materials that can mechanically sustain extreme operating conditions, that may include, among others, high temperature and irradiation. In these environments, it is characteristic that BCC metals (tungsten), display excellent features. Tungsten is the main candidate material to design a Plasma Facing Component (PFCM) for fusion reactors1,2 due to its high melting point, low sputtering yield, and low tritium inventory.3,4 Although the solubility of deuterium in W is low, it can be increased by the sample temperature affecting the formation of defects and vacancies.5 Increasing the defects density even for small amounts of D in the W material6,7,8.

Computational modeling has been used to describe the physical and chemical process of defect production in crystalline W due to ion and plasma irradiation, and mechanical testing9,10 where Molecular Dynamics (MD) simulations have been vastly applied. This numerical approach is highly dependent of the quality of the interatomic potentials that describe the energy of bonding between atoms as a function of atomic coordinates, with the electronic degrees of freedom included only implicitly. For example, large scale MD simulations are mainly based on the embedded atom method (EAM) potentials where the energy of an atomic system is expressed by the sum of pair potential terms of the separation between an atom and the collective chemical bonds between the neighboring atoms.

In this work, we investigate the mechanical nanoindentation response of crystalline W by two interatomic potentials based on embedded atom method (EAM) formalism by Wang et al.11 and Marinica et al.12. The one by Marinica et al., referred as EAM1 in this work, is developed for an investigation of radiation defects as well as dislocations in tungsten. The data set used by EAM1 contains: 1. experimental values such as lattice constant measurements, cohesive energies of tungsten in BCC phase and elastic constants; 2. basic point defects formation energies calculated by ab-initio computations for different crystal orientations of tungsten, namely (100), (110), and (111), interatomic forces for liquid state configurations of tungsten, calculated by means of an ab-initio approach. The resulting EAM potential has been evaluated by comparing with DFT results on point defects (I2 and I4 interstitial clusters as well as two-, three- and four-vacancy clusters formation energy) as well as extended defects (surface energy, Bain deformation energy, dislocation core energy and Peierls energy barrier calculations). The results show that this potential is a good choice for dislocation involved simulations of tungsten, such as nanoindentation measurements.

The latter quality of the EAM1 potential is a good reason for us to use it as a benchmark to model nanoindentation with the Wang et al. potential, defined as EAM2 in this paper, due to the fact that there are several dislocation defects involved in plastic regions in during nanoindentation tests simulations. This EAM2 potential was developed by computing DFT calculation to fit the W-H interactions taken from reported data and generated

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W-W/W-H data by the authors. Here, defect properties like hydrogen with SIA, hydrogen diffusion in strained W are reported in good agreement with DFT calculations. This gives the opportunity to model W-H interaction for further investigation of the effect of deuterium on the dislocation nucleation and dynamics during mechanical testing.

Our paper is organized as follows: In Section 2 we describe the details of the numerical simulations. In Section 3, the atomistic insights of indentation processes in crystalline [111] W sample are presented, where we track hardness, Young’s modulus, and dislocation density as function indentation depth, in conjunction to dislocation loop formation, pile-ups formation showing nanoindentation mechanisms. Finally, in section 4, we provide concluding remarks.

II. COMPUTATIONAL METHODS

In order to perform the MD simulations, we utilize the Large-scale Atomic/ Molecular Massively Parallel Simulator (LAMMPS) software and to model correctly plastic deformation, we first compute the the elastic constants, \( C_{ij} \), bulk modulus, and Poisson’s ratio by two EAM-based interatomic potential for a small BCC W sample of 3.375 nm\(^3\). As well as defect parameters as Energy cohesion for BCC structure, Interstitial energy formation on \(\{111\}\) and \(\{110\}\), and vacancy energy formation that are obtained as:

\[
E^I_{i,v} = E_f - \left[\frac{N_0 \pm 1}{N_0}\right] E_0, \tag{1}
\]

where \(E^I_f\) is the energy formation of interstitial or vacancy; \(E_f\) is the final energy after energy optimization process by considering the interstitial atom or vacancy in the computational cell; \(\pm\) is for interstitial energy and – for vacancy formation energy computation, respectively. The obtained values are presented in Table I. W is a metal that shears in \(\{111\}\) directions on the \(\{110\}\), \(\{112\}\), and \(\{123\}\) planes.

The two EAM-based potentials we utilize are quite similar in most respects, Tab. I. However, a key difference appears in the lattice constant, which is 3.1472 Å for EAM1 \(^{18}\) and 3.16 Å for EAM2 \(^{19}\). Given that the Burgers vector is defined for BCC crystals as \(\vec{b} = a_0 \sqrt{3}/2\), it is clear that the two potentials are expected to have distinct effects on plastic deformation features, such as stacking fault formation and dislocation proliferation. Characteristically, the stacking fault energy scales as \(G \cdot b^2\), while dislocation energies as \(G \cdot b\), suggesting that a fundamental difference in \(b\) should influence and amplify effects that distinguish dislocations from stacking faults during mechanical deformation simulations.

We apply MD simulations through a NVE statistical thermodynamic ensemble to emulate experimental nanoindentation test, where the velocity Verlet algorithm is implemented. Periodic boundary conditions are set on the \(x\) and \(y\) axes to simulate an infinite surface, while the \(z\) orientation contains a fixed bottom boundary and a free top boundary in all MD simulations. We first defined the initial W sample by a size of 31.28 \(\hat{x}\), 32.50 \(\hat{y}\) and 35.58 \(\hat{z}\) with 2 293 200 W atoms followed by a process of energy optimization and equilibration for 100 ps with a Langevin thermostat at 300 K and a time constant of 100 fs. This is done until the system reaches a homogeneous sample temperature and pressure profile with a density of 19.35 g/cm\(^3\) which similar to experimental value. At the first stage, the samples are defined into three sections in the \(z\) direction for setting up boundary conditions along its depth, \(dz\): 1) frozen section with a width of \(\sim 0.02 \times dz\) for stability of the numerical cell; 2) a thermostatic section at \(\sim 0.08 \times dz\) above the frozen one to dissipate the generated heat during nanoindentation; and 3) the dynamical atoms section, where the interaction with the indenter tip modifies the surface structure of the samples. In addition, a 5 nm vacuum section is included at the top of the sample.

The indenter tip is considered as a non-atomic repulsive imaginary (RI) rigid sphere with a force potential defined as: \(F(t) = K \ (\vec{r}(t) - R)^2\) where \(K = 236\) eV/Å\(^3\) (37.8 GPa) is the force constant, and \(\vec{r}(t)\) is the position of the center of the tip as a function of time, with radius \(R = 6\) nm. Here, \(\vec{r}(t) = x_0 \hat{x} + y_0 \hat{y} + (\vec{z}_0 \pm \vec{v}t) \hat{z}\) with \(x_0\) and \(y_0\) as the center of the surface sample on the \(xy\) plane, \(\vec{z}_0 = 0.5\) nm is the initial gap between the surface and the indenter tip moves with a speed \(v = 20\) m/s. The loading and unloading processes are defined by considering the direction of the velocity as negative and positive, respectively. Each process is performed for 125 ps with a time step of \(\Delta t = 1\) fs. The maximum indentation depth is chosen to 3.0 nm to avoid the influence of boundary layers in the dynamical atoms region.

| Parameter       | EAM1 | EAM2 | Exp.       |
|-----------------|------|------|------------|
| \(C_{11}\)      | 522.99 | 522.99 | 501.0      |
| \(C_{12}\)      | 202.99 | 202.99 | 198.0      |
| \(C_{44}\)      | 160.00 | 160.00 | 151.4      |
| Shear Mod.      | 160.0 | 151.47 |
| Poisson R.      | 0.28  | 0.28  | 0.283      |
| Elastic Mod.    | 409.48 | 409.48 | 388.82     |

**Defect properties**

| Value             | EAM1 | EAM2 | DFT |
|-------------------|------|------|-----|
| \(E^\text{coh}\) BCC (eV/atom) | -8.899 | -8.899 | -8.9 |
| \(E^\text{coh}_{\{111\}}\) (eV) | 10.53 | 10.53 | 10.53 |
| \(E^\text{coh}_{\{110\}}\) (eV) | 10.82 | 10.82 | 10.82 |
| \(E^\text{coh}_{\{100\}}\) (eV) | 3.49  | 3.49  | 3.49  |
| \(|b| = a_0 \sqrt{3}/2\) | 2.72 | 2.74 | 2.74 |
A. Oliver-Pharr method

The hardness of the indented sample is calculated by computing the $P - h$ curve with the Oliver and Pharr method[24], following the fitting curve to the unloading process curve as:

$$ P = P_0 (h - h_f)^m $$

with $P$ is the indentation load; $h$ is the indentation depth and $h_f$ is the residual depth after the whole indentation process; and $P_0$ and $m$ are fitting parameters. Thus, the nanoindentation hardness can be computed as: $H = \frac{P_{\max}}{A_c}$ where $P_{\max}$ is the maximum indentation load at the maximum indentation depth, $A_c = \pi (2R - h_c) h_c$ is the projected contact area with $R$ as the indenter tip radius and $h_c = h_{\max} - \epsilon P_{\max}/S$. Here $\epsilon = 0.75$ is a factor related to the spherical indenter shape, and unloading stiffness $S$ is calculated as

$$ S = \left( \frac{dP}{dh} \right)_{h = h_{\max}} = m P_0 (h_{\max} - h_f)^{m-1}. $$

The Young’s module $E_Y$ is computed as:

$$ \frac{1 - \nu^2}{E_Y} = \frac{1}{E_t} - \frac{1 - \nu_t^2}{E_i}. $$

where $\nu$ and $\nu_t$ are the Poisson’s ratio of the Mo sample and indenter, respectively. $E_t$ is the Young’s modulus of the spherical indenter that is considered to be infinitely large, and the effective elastic modulus $E_r = \sqrt{\pi / A_c S} / 2\beta$ with $\beta = 1$ for a spherical indenter shape. In this way, the nano-hardness of the indented samples can be calculated at different temperatures and indenter tip sizes.

B. Dislocation density

In order to analyze the dislocation nucleation and evolution of the sample during mechanical testing, we compute different type of dislocation nucleated at different indentation depth by using OVITO[23] with the DXA package[24], that provides information of the Burgers vector associated to each dislocation. Thus, we categorized the dislocation into several dislocation types according to their Burgers vectors as: $1/2(112)$ and $(001)$ dislocation types. Thus, we compute the dislocation density, $\rho$, as a function of the depth as

$$ \rho = \frac{N_D l}{V_D}, $$

where $N_D$ is the number of dislocation types lines and loops nucleated, $l$ is the dislocation length of each type, and $V_D = 2\pi/3(R_{pl}^3 - h^3)$ is the volume of the plastic deformation region by using the approximation of a spherical plastic zone; where $R_{pl}$ is the largest distance of a dislocation measured from the indentation displacement, considering a hemispherical geometry.

C. Atomic shear strain mapping

For the shear dependence of nanoindentation, atomic strains are computed through the distance difference, $d^2$, between the the $m$-th nearest neighbors of the $n$-th atom of the pristine and indented samples. Followed by defining the Lagrangian strain matrix of the $n$-th atom as[7] :

$$ \eta_n = \frac{1}{2} \left( J_n J_n^T - I \right), $$

with

$$ J_n = \left( \sum_m d_m^{iT} d_m^i \right)^{-1} \left( \sum_m d_m^{iT} d_m^i \right). $$

Thus, the shear invariant of the $n$-th atom is computed as:

$$ \eta_n = \sqrt{\zeta_{ij} \zeta_{ij}} / 2, \text{ with } \zeta_{ij} = \eta_{ij} - \eta_{jk} \delta_{ij}. $$

This approach is implemented in OVITO[23].

III. RESULTS

The loading and unloading process of nanoindentation test of W sample is recorded and shown in Fig. 1. We include a Hertz fitting curve based on the sphere-flat surface contact and expressed as $P_t = \frac{3}{4} E_{eff} R^{1/2} h^{3/2}$, where $R$ is the indenter radius, $h$ is the indenter displacement, and $E_{eff}$ is the elastic modulus; to show the plastic deformation transition during the loading process by the identification of the first pop-in event (inset figure). Here, W-W and W-H potentials agreed with this mechanical process. However, the W-W models more pop-in events during the loading process than the W-H simulation. Nevertheless, both approaches report the same...
value for the maximum load at the maximum indentation depth. The unloading process is commonly used to calculate the Hardness and Young’s modulus of the material by Oliver-Pharr method, where both simulations present similar results, albeit of the recombination effects observed at 2 nm depth by the EAM1 simulations. The reduced Young’s modulus computed by Oliver-Pharr method is 173.78 GPa and 172.65 GPa, for the EAM1 and EAM2 potentials, respectively.

### A. Dislocation nucleation and evolution

In general, dislocation glide occurs in the closest-packed (111) directions for BCC metals with Burgers vector \( b = \frac{1}{2}(111) \), and slip planes belong to the \{110\}, \{112\} and \{123\} families. To analyze the atomic structure during nanoindentation test which provides information about the mechanisms of dislocation nucleation and evolution, we compute and visualization of the dislocation structure at different indentation depths by using the Dislocation Extraction Analysis (DXA) tool. The output data provides the total length of dislocation lines and loops and their corresponding Burgers vectors.

![Dislocation density vs indentation depth](image)

**FIG. 2.** (Color on-line). Total, \( \frac{1}{2}(111) \) type, and \( (100) \) type dislocation density as a function of the indentation depth obtained by both approaches. Dislocation nucleation mechanisms are described differently by both interatomic potentials, where a single prismatic loop is nucleated at 2nm depth.

Thus, computed dislocation density as a function of the indentation depth is reported in Fig. 2.

We analyze the dislocation nucleation during nanoindentation test by tracking the total and main dislocation types with Burgers vector \( \frac{1}{2}(111) \) and \( (100) \) that are observed. Both approaches show oscillations of the dislocation density during the loading process, and the identified drop minimum at 2nm depth is related to the nucleation of a single prismatic loop. At the end of the indentation test, labeled as unload in Fig 2, the total dislocation density decreases reaching a value of \( 1.5 \times 10^{-12} \) cm\(^{-2} \) due to the recovery of the sample. During the unloading of the indenter tip, the \( 1/2(111) \) dislocations are absorbed by the surface due to recrystallization mechanisms of W.

It is noted that EAM1 and EAM2 potentials model the dynamics of the elastic to plastic deformation transition differently. At a depth of 0.8 nm, a half loop is nucleated by EAM1 half loops with a Burgers vector \( 1/2(111) \) produces a \( (100) \) junction was nucleated by EAM2 potentials, as shown in Fig. 3. However, the lasso-like dislocation is nucleated by both approaches at 2nm depth where the single prismatic loop is nucleated (Fig 3). From 2nm to 3nm depth, both MD simulations model the evolution of a single loop but at different mobility rates. Interestingly, during the unloading process the shear single loop is absorbed by the dislocation network in a reverse mechanism for the EAM2 simulations. While the EAM1 simulation describes the loop dynamics in a different way, the dislocation network underneath the indenter tip is mainly absorbed by the surface leaving the loop oscillating at a depth of 12 nm respect to the sample surface. This is the main difference between the MD simulations performed by two different approaches.

It is well known that dislocation glide in BCC metals is mainly governed by the Peierls barrier, which measures the stress that needs to be applied in order to move a dislocation core to the next atomic valley in the glide plane. Thus, the ‘lasso’ mechanism is observed by both methods, suggesting that the main dislocation nucleation mechanism remains analogous to other BCC metals. Moreover, the Peierls barrier is smaller for edge dislocations than for screw dislocations, where the BCC metal plasticity is dominated by the sluggish glide of screw dislocation segments, as shown by our MD simulations. The visualization of the dislocation dynamics during nanoindentation test by both approaches is reported in the supplementary material of this paper.

In order to compare the results obtained by both EAM potentials, we compute the number of Frenkel pair (FP) formed as a function of the indentation depth by Wigner-Seitz method, as visualized in Fig. 3 and shown in Fig. 4. At a indentation depth of 0.8 nm, both approaches show a similar shaped FP region regardless the type of the nucleated dislocations. The difference in the dynamics of FP production started at a depth of 2 nm, where their propagation follows the \([10-1]\), \([01-1]\), and \([1-12]\) slip planes for the EAM2 potentials while this effect is not fully observable for the EAM1 potentials. At the

\[ \text{Dislocation density (x10^4 m}^{-2} \) \]
maximum indentation depth (3 nm); the FP formation clearly follows the slip system family for BCC metal into a defined plastic region for the EAM2, contrasting the evolution of FP formation for the EAM1 potentials where the plastic region under the tip is not well defined by the MD simulation. These mechanisms lead to different recovery of the W sample modeled by both approaches.

The quantification of FP creation as a function of the indentation depth (see Fig. 4) shows the same trend for both approaches. However, by computing the difference of FP results as reported in the inset of Fig. 4, one observes that the dynamics of FP formation differs when the shear dislocation loop is nucleated during the loading process. Here, the EAM2 potentials modeled this dynamics in a better way than EAM1 due to the parametrization for the EAM1 potentials collision cascades.

B. Pile ups formation

MD simulations results can be compared to Scanning electron microscopy (SEM) images in a qualitative way by analyzing the indenter mark left by the tip after nanoindentation and at the maximum indentation; where the former is inaccessible in the experiments. For this reason, we compute the displacement atoms of the indented sample by comparing to the pristine one where pileups formation can be characterized. In Fig. 5 we show results for the pileups formation at the maximum indentation depth and after unloading process by both approaches.

The slip traces marks on the surface of the W sample are clear evidences from crystal plasticity. This phenomena indicates the underlying dislocation glide mechanisms during nanoindentation testing. The interaction of slip traces causes different patterns on the surface (pile up patterns) which are heavily crystalline orientation dependent. Here, pile up morphology for a (111)-oriented BCC W has a three-fold pile up pattern as shown by our results for atomic displacement on the z axis. Figure 5 vividly shows that this fact is quite true for

FIG. 3. (Color on-line). Visualization of the dislocation nucleation and evolution at different indentation depths and after unloading the tip by both approaches. As well as identified Frenkel pair during nanoindentation test depicted as red spheres. A shear dislocation loops is nucleated at the maximum indentation depth by both potentials.

FIG. 4. (Color on-line). Number of Frenkel Pairs formed as a function of the indentation depth computed by Wigner-Seitz method. Difference of numbers between the EAM potentials are presented in the inset.
our investigations for both interatomic potentials. Also, Varilla et al. investigated nanoindentation pile up patterns for Ta oriented in (111) directions. Although the temperature of their simulation (77 K) and their indenter radius (24 nm) is different to our calculations, the pile up patterns they reported is similar to ours due to the BCC geometry of W samples.

C. von Mises strain mapping

In Fig 6 we present the computed von Mises strain mapping at the maximum indentation depth and after unloading process for EAM2 in a) and EAM1 in b) potentials. The sample is slid to the half on the \{111\} plane to visualize the atomic distribution of the shear strain by coloring W atoms according to their values, where maximum strain is observed underneath the indenter tip. We noticed that the majority of the observed slip traces in the MD simulations are characterized by limited mobility of the screw dislocation segments that is also observed by the strain mapping. This fact is considered to be a key to the development of the defect network and to the onset of surface slip traces; during loading process.

For the unloading process, EAM2 potentials model the recovery of the material by absorbing the dislocation loop, while the EAM1 potentials present a stable loop after nanoindentation test identified by the green colored strain lines.

IV. CONCLUDING REMARKS

In this work, MD simulations by using two different EAM-based interatomic potential are performed to investigate the nanomechanical response of crystalline W oriented to [111] during nanoindentation test. We analyzed the dislocation nucleation and evolution mechanisms described by both approaches. We characterized the nanoindentation process in W by tracking shear strain accumulation and displacement atoms mapping that can be compared to SEM investigations. We can summarize our work as follows: 1) the comparison between the potentials reports similarities for the recorded load displacement curves, hardness and young’s modulus of the W sample, as well as the rosettes formed at the surface projections of the preferential gliding direction during nanoindentation; 2) dislocation nucleation mechanisms are modeled in a different way during nanoindentation test due to difference of the Burgers vector magnitude related to stacking fault formation and dislocation dynamics. Although a prismatic loop is nucleated by both approaches, the dynamics is completely different where the loop has a reserve process for the parametrization of W-H. Based on the present results, we conclude that nanoindentation test can be modeled by several interatomic potentials where the load displacement graph can be similar. However, dislocation dynamics depends on the approach used to developed the MD potentials where Transmission electron microscopy investigation can help to the numerical modeling. These results also open an opportunity to study dislocation nucleation mechanism in hydrogenated W samples.

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and its supplementary material.

DATA AVAILABILITY STATEMENT

The raw data and MD simulations results and nanoindentation tests of W sample visualization that support the findings of this study are available within the article and its supplementary material.

1. M. Rieth, J. Bourtard, S. Dudarev, T. Ahlgren, et al., Journal of Nuclear Materials 417, 463 (2011).
2. P. Pamela, A. Bécoulet, D. Borba, J.-L. Bourtard, L. Horton, and D. Maisonnier, Fusion Engineering and Design 84, 194 (2009).
3. N. Holtkamp, Fusion Engineering and Design 84, 98 (2009).
4. M. Mayer, M. Andrzejczuk, R. Dux, E. Fortuna-Zaleska, A. Hakola, S. Koivuranta, K. Krieger, K. J. Kurzydlowski, J. Likonen, and G. Matern, Physica Scripta T138, 014039 (2009).
5. P. Piaggi, E. Bringa, R. Pasionat, N. Cordillo, M. Panizo-Laiz, J. del Río, C. G. de Castro, and R. Gonzalez-Arrabal, Journal of Nuclear Materials 458, 233 (2015).
6. B. Lipschultz et al., Technical Report MIT PSFC/RR, 10 (2010).
7. M. Kaufmann and R. Neu, Fusion Engineering and Design 82, 521 (2007).
8. K. Heinola, T. Ahlgren, K. Nordlund, and J. Keinonen, Phys. Rev. B 82, 094102 (2010).
9. E. Hodille, S. Markelj, T. Schwarz-Selinger, A. Založnik, M. Pečovnik, M. Kelemen, and C. Grisolia, Nuclear Fusion 59, 016011 (2018).
10. P. Schwarz-Selinger, J. Bauer, S. Elgeti, and S. Markelj, Nuclear Materials and Energy 17, 228 (2018).
11. Y.-N. Liu, T. Ahlgren, L. Bukonte, K. Nordlund, X. Shu, Y. Yu, X.-C. Li, and G.-H. Lu, AIP Advances 3, 122111 (2013).
12. D. R. Mason, D. Nguyen-Manh, M.-C. Marinica, R. Alexander, A. E. Sand, and S. L. Dudarev, Journal of Applied Physics 120, 075112 (2019).
13. T. Ahlgren, K. Heinola, N. Juslin, and A. Kuronen, Journal of Applied Physics 107, 035156 (2010).
14. T. Byggmåstar, A. Hamedani, K. Nordlund, and F. Djurabekova, Phys. Rev. B 100, 144105 (2019).
15. K. Nordlund, S. Zinkle, A. Sand, et al., “Improving atomic displacement and replacement calculations with physically realistic damage models.” (2018).
16. M.-C. Marinica, L. Ventelon, M. R. Gilbert, L. Proville, S. L. Dudarev, J. Marian, G. Bencetux, and F. Willaime, Journal of Physics: Condensed Matter 25, 395502 (2013).
17. L.-F. Wang, X. Shu, G.-H. Lu, and F. Gao, Journal of Physics: Condensed Matter 29, 435401 (2017).
18. S. Goel, G. Cross, A. Stukowski, E. Gansjäger, B. Beake, and A. Agrawal, Computational Materials Science 152, 196 (2018).
19. A. P. Thompson, H. M. Aktulga, R. Berger, D. S. Bolintineanu, W. M. Brown, P. S. Crozier, P. J. in’t Veld, A. Kohlmeyer, S. G. Moore, T. D. Nguyen, R. Shan, M. J. Stevens, J. Tranchida, C. Trott, and S. J. Plimpton, Computer Physics Communications 271, 108171 (2022).
20. W. R. Hertzberg and F. E. Hauser, (1977).
21. F. Dominguez-Gutiérrez, S. Papanikolaou, A. Esfandiarpour, P. Sobkowicz, and M. Alava, Materials Science and Engineering: A 826, 141912 (2021).
22. W. Oliver and G. Pharr, Journal of Materials Research 7, 1564–1583 (1992).
23. A. Stukowski, Modelling and simulation in materials science and engineering 18 (2010), 10.1088/0965-0393/18/1/015012.
24. A. Stukowski, V. V. Bulatov, and A. Arsenlis, Modelling and Simulation in Materials Science and Engineering 20, 085007 (2012).
25. A. D. Backer, D. Mason, C. Domain, D. Nguyen-Manh, M.-C. Marinica, L. Ventelon, C. Bœcquat, and S. Dudarev, Nuclear Fusion 58, 016006 (2017).
26. K. Nibur and D. Bahr, Scripta Materialia 49, 1055 (2003).
27. S. Harvey, H. Huang, S. Venkataraman, and W. Gerberich, Journal of Materials Research 8, 1291 (1993).
28. E. Renner, Y. Galliard, F. Richard, F. Amiot, and P. Delobelle, International Journal of Plasticity 77, 118 (2016).
29. S. Pathak, J. L. Riesterer, S. R. Kalidindi, and J. Michler, Applied Physics Letters 105, 161913 (2014).
30. M. M. Biener, J. Biener, A. M. Hodge, and A. V. Hamza, Phys. Rev. B 76, 16522 (2007).
31. J. Varillas-Delgado and J. Alcala Cabrelles, A molecular dynamics study of nanoncontact plasticity and dislocation avalanches in FCC and BCC crystals, PhD dissertation, Universitat Politècnica de Catalunya. Departament de Ciència dels Materials i Enginyeria Metal·lúrgica (2019).
32. V. Wang, D. Raabe, C. Klaiber, and F. Roters, Acta Materialia 52, 2229 (2004).
33. Y. Liu, S. Varghese, J. Ma, M. Yoshino, H. Lu, and R. Komanduri, International Journal of Plasticity 24, 1990 (2008).