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a. REPORT	b. ABSTRACT	c. THIS PAGE			Douglas Spearot
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RPPR Final Report
as of 04-Aug-2021

Agency Code: 21XD

Proposal Number: 70354MS **Agreement Number: W911NF-17-1-0194**
INVESTIGATOR(S):

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Report Date: 31-Aug-2021 Date Received: 03-Aug-2021
Final Report for Period Beginning 01-May-2017 and Ending 31-May-2021

Title: Virtual Diffraction Techniques used to Study Dislocation Loop ? Grain Boundary Interactions and Assess Slip Transfer Criteria
Begin Performance Period: 01-May-2017 **End Performance Period:** 31-May-2021
Report Term: 0-Other

Submitted By: Douglas Spearot Email: dspearot@ufl.edu
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STEM Degrees: 2 **STEM Participants:** 3

Major Goals: The overarching objective of this project is to develop a multiscale simulation approach to investigate dislocation – grain boundary interactions and to employ this approach to advance criteria for slip transfer across grain boundaries to include the grain boundary damage state. Existing atomistic simulation approaches to study dislocation – grain boundary interactions, where an atomistic model of an infinitely long (periodic) edge or screw dislocation is forced to interact with a grain boundary at high driving stress, are not sufficient to resolve the multiscale nature of dislocation core absorption, decomposition and slip transfer. Furthermore, existing discrete dislocation dynamics (DDD) simulations do not consider the stress state of a grain boundary (GB) and its effect on slip transfer. This work introduces a different atomistic approach based on the use nanoscale dislocation loops and proposes a disclination based approach to incorporate residual dislocation content into DDD simulations.

Over the project period, the following technical goals were defined:

(1) Compute important properties related to dislocation core structure, Peierls barriers and dislocation mobility as a function of dislocation character angle and local stress state using atomistic simulations. Importantly, the role of local stress state must be considered because as a dislocation approaches another dislocation or a grain boundary, the interaction stresses are significant and these can affect core structure.

(2) Incorporate dislocation related data from atomistic simulations into DDD simulations and perform validation simulations to confirm that DDD is capable of reproducing dislocation behaviors observed in atomistic simulations. This includes character angle dependent and stress state dependent dislocation mobilities. When provided to DDD simulations, this information provides more realistic dislocation kinetics, so that the behavior of a straight dislocation or dislocation loop moving within the stress field created by other defects is more accurately reproduced.

(3) Investigate the influence of atomistically motivated dislocation kinetics on the plastic path taken by a network of dislocations during deformation. Specific differences in the stress-strain relationships are to be correlated with evolution of the dislocation network with different models for dislocation mobility.

(4) Implement a model for the stress field of grain boundaries and a technique to perform dislocation transmission within the DDD simulation code. These advancements will allow for a study of the role of grain boundary stress field on dislocation transmission including the evolution of the residual dislocation on the grain boundary.

(5) Develop and implement a model for the evolution of the mechanical state of a grain boundary due to prior dislocation transmission events. This model is intended to explore dislocation transmission through grain boundaries with “damage” from prior slip transfer events. With this model, explore the transmission strength of a grain boundary as a function of the number and type of prior dislocation transmission events.

(6) For analysis and bridging to atomistic simulations and experiments, develop a new virtual diffraction algorithm for DDD simulations that overcomes inaccuracy and computational cost limitations of prior methods [1]. This was done in collaboration with staff at Los Alamos National Laboratory staff (Capolungo and x-ray diffraction experimentalists). Specifically, this new algorithm was used to generate data necessary for a data-driven approach to predict dislocation densities from x-ray diffraction peak broadening.

Over the project period, the following workforce and dissemination goals were defined:

(1) Train and mentor Ph.D. students. Three Ph.D. students were supported by this award over the project period. Dr. Khanh Dang completed his Ph.D. in 2018 on the use of atomistic simulations to study individual dislocation behaviors and generate databases of dislocation properties for use in DDD simulations. Dr. Darshan Bamney completed his Ph.D. in 2021 on the use of DDD simulations to study slip transfer and the role of grain boundary mechanical state. He incorporated data from Dr. Khanh Dang into his DDD code. Mr. Royce Reyes performed atomistic simulations of dislocation loop interaction with grain boundaries in aluminum. He worked closely with Dr. Darshan Bamney to model grain boundaries relevant to the DDD simulation studies. Full details are provided in the “Training Opportunities” section.

(2) Involve undergraduate students through academic year research experiences. Three undergraduate students participated in this research. Full details are provided in the “Training Opportunities” section.

(3) Disseminate research results. Multiple journal publications and research presentations at professional meetings/conferences were produced from the research results. Full details are provided in the “Results Dissemination” section.

Accomplishments: Overall, the research supported by this award has significantly advanced the ability to study and predict polycrystalline plasticity using discrete dislocation dynamics simulations.

Figures 1-3 show results for the behavior of dislocation loops as a function of size and the parameterization of DDD simulations using lattice friction stress and core width parameters derived from or motivated by atomistic simulations [2]. Figure 1 presents the static (0 K) shear stress necessary for dislocation loop equilibrium for several interatomic potentials tested, with comparison to the Scattergood and Bacon equation [3]. Figure 2(a) shows the effect of temperature on the resolved shear stress necessary for dislocation loop stability using the Zope and Mishin Al potential [4]. This figure shows that temperature lowers the minimum resolved shear stress necessary to open a dislocation loop and that the differential between resolved shear stresses at a given dislocation loop size becomes smaller with increasing temperature. This provides a measurement of the decay in the effective lattice friction stress as a function of temperature, leading to the proposed Eq. (1). Figure 2(b) shows that the effective lattice friction stress decreases as a function of temperature for all dislocation loop sizes. A size dependence is apparent, which is prominent for dislocation loops smaller than 16.2 nm in radius. An optimal DDD core width parameter is determined which best fits DDD simulation results to the atomistic simulation data. Examples of this fitting at 300 and 400 K are shown in Fig. 3. An excellent fit is attained for dislocation loops above the critical radius of 16.2 nm.

In addition to the above calibration of the core width parameter, molecular dynamics (MD) simulations are used to compute the mobility of screw, 30 degree, 60 degree, and edge straight dislocations under different Schmid stresses, different combinations of Escaig stress, and different stresses normal to the (111) slip plane [5,6]. Examples of data for screw dislocations are shown in Figs. 4 and 5 with fits to the data provided by Eq. (2). The dislocation mobility laws determined from atomistic simulations are implemented into a nodal DDD model. A four-dimensional linear interpolation scheme is used to determine the linearized coefficient that describes the current relationship between nodal velocity for a dislocation segment of arbitrary character angle moving under the influence of a generalized stress state.

The ability of the atomistically informed DDD framework to accurately model complex dislocation geometries is verified by considering the expansion of a nanoscale dislocation loop [6]. Figures 6(a) and 6(b) show snapshots of

the evolution of the dislocation loop geometry compared against MD loop expansion data for tau_e= 250 MPa and sigma_n=500 MPa, respectively. Overall, DDD results are in good agreement with atomistic data, and the DDD model is capable of replicating the essential features of the loop geometry accurately. Then, the evolution of dislocation networks using atomistically informed dynamics described by two different mobility laws is investigated [6]. The first mobility law describes the force-velocity relationship in the linear and non-linear regimes as a function of dislocation character angle only [5]; this is referred to as the “character angle law”. The second mobility law includes both character angle and local stress state dependence and is denoted as the “full mobility law” [6]. For a dislocation network with starting dislocation density of rho_o = 1.56x10^13 m^-2 distributed on 8 different slip systems, Fig. 7 shows the microstructures at different axial strains with different mobility law assumptions are visually different. The engineering stress-strain response and the dislocation density profiles are shown in Figs. 8 (a) and 8(b), respectively. In the stress-strain curves, the magnitudes of the stress drop are found to be appreciably different for the networks evolving according to the two different mobility laws. The stress drops in the networks studied here are directly linked to increases in glissile dislocation activity [7].

Next, a novel approach is developed to investigate the influence of intergranular stresses induced by equilibrium and non-equilibrium grain boundaries (EGBs and NEGBs) on dislocation transmission within DDD simulations [8]. Specifically, a disclination-based framework is used to describe the equilibrium intergranular stress fields of select symmetric tilt GBs, as shown in Fig. 9(a). Then, slip transfer through these GBs is simulated via an algorithm that predicts dislocation transmission considering geometric and plastic dissipation criteria. Results show that the locations for dislocation transmission are strongly correlated with the GB stresses, as shown in Fig. 10 for a specific symmetric tilt GB. In addition, the glide of residual dislocations on the GB plane is also strongly influenced by the stress field of the disclination dipoles used to describe the GB structure, as shown in Fig. 11. In a first approach to approximate GB damage due to prior slip transfer, ordered structural defects in the equilibrium GBs are modified via the incorporation of extrinsic grain boundary dislocations, resulting from the decomposition of the residual on the GB, which is illustrated in Fig. 9(b). This creates long range stress fields at the GB, and slip transfer preferentially initiates near the nonequilibrium defects, as shown in Fig. 12.

Next, a more general approach to investigate the role of prior slip transmission on the critical shear stress necessary for subsequent slip transfer is developed by advancing the concept of incorporation of dislocation content into disclination dipoles [9]. Figure 13 shows a schematic of the complete model, which accounts for (i) time increments between arriving dislocation loops at the GB, (ii) the creation of residual dislocation content over the length of the slip trace for the first dislocation transmission event, and (iii) the buildup of the residual dislocation content along the slip trace for multiple dislocation transmission events. Figure 14 shows the effect of prior dislocation slip transmission on subsequent slip transfer. The driving stress ratio is defined as the resolved shear stress on the outgoing slip system necessary for slip transmission, normalized by the reference value for an equilibrium grain boundary. DDD simulations predict that the barrier strength of the GB to dislocation transmission decreases with the areal density of absorbed GB dislocations. Importantly, the reduction in the barrier strength of the GB is not simply due to changes in the resolved shear stress on the transmission slip system, as shown in Fig. 15. This would be the result predicted using classical slip transmission models [10,11]; instead, the DDD simulations in this work shows that the resolved shear stress on the residual dislocations within the GB plane is critical, as this driving stress helps de-pin the residual and the transmitted dislocation, which allows the transmitted embryo to grow in the transmission grain. Complete details of this model and analysis can be found in [9].

Finally, a new method to generate virtual diffraction patterns from dislocated crystals in DDD simulations is developed [14]. This technique leverages a full-field spectral computation of the elastic strain fields generated in the presence of an ensemble of dislocations. The new DDD diffraction algorithm is based on the imperfect crystal model detailed in Warren [12] and is designed to work in conjunction with the DDD-FFT framework of Bertin et al. [13]. Figure 16 shows diffraction profiles from a network of dislocations using strain correlation independent (Stokes-Wilson) and strain correlation dependent (L-dependent) approaches.

Training Opportunities: Over the duration of the project, this award supported the training and mentorship of three Ph.D. students at the University of Florida: Dr. Khanh Dang, Dr. Darshan Bamney and Mr. Royce Reyes. In addition, several undergraduate students participated in this research through academic year research experiences.

Dr. Khanh Dang completed his Ph.D. in the summer of 2018. He is currently a Post Doc at Los Alamos National Laboratory, and he is in the process of converting to a full Member of the Technical Staff in the Materials Science and Technology Division. Dr. Dang was trained on atomistic simulations and was responsible for all simulations associated with individual behaviors of dislocations in Al. Specifically, this included (i) calculations of Peierls stress for dislocations as a function of character angle and stress state, (ii) measurement of dislocation mobilities as a function of character angle and stress state, and (iii) construction of dislocation loops and measurement of the shear stress necessary for loop stability. This data was used as input to DDD or to calibrate output of DDD simulations.

Dr. Darshan Bamney completed his Ph.D. in the summer of 2021. He will be starting as a Post Doc at Los Alamos National Laboratory later in 2021. Dr. Bamney was trained to perform discrete dislocation dynamics simulations using high performance computers with GPUs. In addition, Dr. Bamney has become an expert in the description of grain boundaries using continuum mechanics fields. During the summer of 2018 and the summer of 2019, Dr. Bamney worked at Los Alamos National Laboratory with Dr. Capolungo and his research group to advance the DDD code to meet the objectives of this project.

Mr. Royce Reyes is a Graduate Research Assistant at the University of Florida. He is of Hispanic descent and completed his undergrad degree in Mechanical Engineering at the University of Florida. Mr. Reyes underwent training in (1) high-performance computing usage, (2) atomistic simulations including molecular statics, molecular dynamics techniques, and (3) analysis of atomistic scale structures using virtual diffraction methods. He worked closely with Dr. Bamney to model using atomistic simulations the same grain boundaries as were selected for study in the DDD simulations.

During the 2017-2018 academic year, Materials Science & Engineering undergraduate student Mr. Kanis Bootsita joined the research team, in partnership with the University Scholars Program at the University of Florida. Mr. Bootsita learned how to conduct molecular dynamics simulations and contributed results of the role of interatomic potential on the mobility laws for edge and screw dislocations. During the 2018-2019 academic year, Mechanical & Aerospace Engineering undergraduate student Mr. Nicolas Mabilleau joined the research team. Mr. Mabilleau learned how to conduct DDD simulations working with Dr. Bamney. During the 2020-2021 academic year, Mechanical & Aerospace Engineering undergraduate student Mr. Joshua Kempfert joined the research team. He learned how to perform atomistic simulations and will continue his work in the 2021-2022 academic year on the mobility of residual dislocations on grain boundaries.

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Results Dissemination: Project results have been disseminated via multiple outlets. The journal paper listed as "under review" is currently under first review at the journal indicated. The journal paper listed as "in preparation" is in the final stages of writing and will be submitted before the end of 2021.

Journal Papers Published during Project Lifetime:

[1] Dang, K.Q., Capolungo, L., Spearot, D.E. (2017) Nanoscale dislocation shear loops at static equilibrium and finite temperature, Modeling and Simulation in Materials Science and Engineering, 25, 085014.

[2] Dang, K.Q., Spearot, D.E. (2018) Pressure dependence of the Peierls stress in aluminum, JOM, 70, 1094-1099.

[3] Dang, K.Q., Bamney, D., Bootsita, K., Capolungo, L., Spearot, D.E. (2019) Mobility of dislocations in aluminum: Faceting and asymmetry during nanoscale dislocation shear loop expansion, Acta Materialia, 168, 426-435.

[4] Kacher, J., Pierron, O., Zhu, T., Spearot, D.E. (2019) Integrating in situ TEM experiments and atomistic simulations for defect mechanics, Current Opinions in Solid State & Materials Science, 23, 117-128.

[5] Bamney, D., Tallman, A., Capolungo, L., Spearot, D.E. (2020) Virtual diffraction analysis of dislocations and dislocation networks in discrete dislocation dynamics simulations, Computational Materials Science, 174, 109473.

[6] Dang, K.Q., Bamney, D., Capolungo, L., Spearot, D.E. (2020) Mobility of dislocations in aluminum: Role of non-Schmid stress state, Acta Materialia, 185, 420-432.

[7] Bamney, D., Capolungo, L., Spearot, D.E. (2021) Role of equilibrium and non-equilibrium grain boundary stress fields on dislocation transmission, Journal of Materials Research, 36, 2687-2704.

Journal Papers Under Review or Currently in Preparation:

[8] Tallman, A., Pokharel, R., Bamney, D., Spearot, D.E., Lebensohn, R., Brown, D., Capolungo, L. (2021) Data-driven analysis of neutron diffraction line profiles: Application to plastically deformed Ta, NPJ Computational Materials, under review.

[9] Bamney, D., Reyes, R., Capolungo, L., Spearot, D.E. (2021) Grain boundary stress field evolution due to dislocation-grain boundary interactions and effect on subsequent dislocation transmission, Journal of the Mechanics and Physics of Solids, in preparation.

Conference and Invited Seminar Presentations during Project Lifetime:

[1] Dang, K., Capolungo, L., Spearot, D.E. (2017) Nanoscale dislocation shear loops at static equilibrium and finite temperature via atomistic simulations, presented at: ASME IMECE, Tampa, FL.

[2] Dang, K., Capolungo, L., Spearot, D.E. (2018) Algorithm to simulate the structure and mobility of nanoscale dislocation shear loops via atomistic simulations, presented at: TMS Annual Meeting, Phoenix, AZ.

[3] Spearot, D.E. (2018) Integration of atomistic and discrete dislocation dynamics simulations for modeling dislocations and dislocation – defect interactions, presented at: U.S. Army Research Laboratory, Aberdeen, MD. [Invited]

[4] Spearot, D.E. (2018) Development of virtual diffraction techniques for atomistic simulations with application to dislocations and grain boundaries, presented at: Georgia Institute of Technology, Atlanta, GA. [Invited]

[5] Bootsita, K., Dang, K.Q., Spearot, D.E. (2018) Comparison of molecular dynamics interatomic potentials in the prediction of dislocation mobility, presented at: UF Undergraduate Research Symposium, Gainesville, FL.

[6] Dang, K., Capolungo, L., Spearot, D.E. (2018) Atomistic simulation of dislocation properties in Aluminum for parameterization of discrete dislocation dynamics models, presented at: U.S. National Congress on Computational Mechanics, Chicago, IL.

[7] Dang, K., Bamney, D., Bootsita, K., Capolungo, L., Spearot, D.E. (2018) Atomistic simulation of dislocation properties in Al for parameterization of discrete dislocation dynamics models, presented at: Society for Engineering Science Meeting, Madrid, Spain.

[8] Spearot, D.E., Dang, K. (2019) Atomistic simulation methods for computing character angle and stress-state dependent dislocation properties, presented at: TMS Annual Meeting, San Antonio, TX. [Invited]

[9] Bamney, D., Tallman, A.E., Capolungo, L., Spearot, D.E. (2019) Virtual diffraction analyses of microstructural features in discrete dislocation dynamics simulations, presented at: TMS Annual Meeting, San Antonio, TX.

[10] Spearot, D.E. (2019) Atomistic simulations of dislocation loop geometry and mobility for parameterization of discrete dislocation dynamics simulations, presented at: Sandia National Laboratories, Albuquerque, NM. [Invited]

[11] Bamney, D., Dang, K.Q., Capolungo, L., Spearot, D.E. (2020) Hierarchical integration of atomistically derived dislocation mobility laws into discrete dislocation dynamics simulations, presented at: TMS Annual Meeting, San Diego, CA.

[12] Tallman, A., Bamney, D., Spearot, D.E., Capolungo, L. (2020) Revisiting the Wilkens function: A discrete dislocation dynamics based study of diffraction strain broadening, presented at: TMS Annual Meeting, San Diego, CA.

[13] Spearot, D.E., Dang, K., Bamney, D., Capolungo, L. (2020) Importance of dislocation character angle and local stress state dependent mobility laws on discrete dislocation dynamics modeling of plasticity in aluminum, presented at: DPG Spring Meeting, Dresden, Germany. [Invited] [Cancelled due to COVID-19]

[14] Bamney, D., Dang, K.Q., Capolungo, L., Spearot, D.E. (2020) Hierarchical multiscale study of the role of dislocation mobility on plasticity in aluminum, presented at: Society for Engineering Science (SES) Meeting. [Virtual]

[15] Spearot, D.E. (2020) Modeling plasticity in metals at atomistic and mesoscopic length scales, presented at: Conference on Processing and Characterization of Materials (CPCM 2020), Rourkela, India. [Invited] [Virtual]

[16] Bamney, D., Capolungo, L., Spearot, D.E. (2021) Advancements in discrete dislocation modeling of slip transmission through equilibrium and non-equilibrium grain boundaries, presented at: TMS Annual Meeting. [Virtual]

[17] Reyes, R., Spearot, D.E. (2021) Dislocation pileup induced transmission across grain boundaries in aluminum via molecular dynamics simulations, presented at: TMS Annual Meeting. [Virtual]

Honors and Awards: Dr. Khanh Dang received the Best Ph.D. Dissertation in the Solid Mechanics, Design and Manufacturing division of the Department of Mechanical & Aerospace Engineering at the University of Florida. His dissertation was titled “Atomistic Simulations of Dislocation Properties and the Role of Stress State in Aluminum.”

Dr. Darshan Bamney was named as a recipient of the Outstanding Achievement Award for research from the Herbert Wertheim College of Engineering at the University of Florida. This award recognizes outstanding contributions of international students to promote and foster advancement of the research community in the College of Engineering at UF.

Project PI Dr. Douglas Spearot was promoted to the rank of Professor in the Department of Mechanical & Aerospace Engineering at the University of Florida in 2020. In addition, the PI received the TMS Manufacturing and Materials Processing Division (MPMD) Distinguished Service Award in 2020. This award recognizes contribution to the operation of MPMD in the TMS Professional Society.

Protocol Activity Status:

Technology Transfer: The computational tools developed in this research program can be extended to other areas of research and to different material systems. In a collaboration with Brigham Young University (Homer), the atomistic virtual diffraction algorithm, and the method to generate dislocation loops, were extended so that Kikuchi diffraction patterns could be predicted. In addition, the tools can be applied to HCP materials systems to explore dislocation behaviors and other related plastic deformation phenomena. This has begun via informal collaboration with staff members at Los Alamos National Laboratory, resulting in two papers (in addition to those that are directly related to this award discussed previously). Several presentations were given at national meetings related to this complementary project.

[1] Herron, A.D., Coleman, S.P., Dang, K.Q., Spearot, D.E., Homer, E.R. (2018) Simulation of kinematic Kikuchi diffraction patterns from atomistic structures, MethodsX, 5, 1187-1203.

[2] Spearot, D.E., Capolungo, L., Tome, C.N. (2019) Shear driven motion of Mg {10-12} twin boundaries via disconnection terrace nucleation, growth and coalescence, Physical Review Materials, 3, 053606, 1-9.

[3] Spearot, D.E., Taupin, V., Dang, K.Q., Capolungo, L. (2020) Structure and kinetics three-dimensional defects on the {10-12} twin boundary in magnesium: Atomistic and phase-field simulations, Mechanics of Materials, 143, 103314.

In 2020, Los Alamos National Laboratory provided Spearot a subaward to advance atomistic and DDD simulation capabilities to study dislocation transmission at Al/Fe FCC/BCC interfaces. The techniques and methods developed in the current project are being used in this new effort.

PARTICIPANTS:

Participant Type: PD/PI
Participant: Douglas Spearot
Person Months Worked: 1.00 **Funding Support:**
Project Contribution:
National Academy Member: N

Participant Type: Graduate Student (research assistant)
Participant: Khanh Dang
Person Months Worked: 6.00 **Funding Support:**
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National Academy Member: N

Participant Type: Graduate Student (research assistant)
Participant: Darshan Bamney
Person Months Worked: 6.00 **Funding Support:**
Project Contribution:
National Academy Member: N

Participant Type: Graduate Student (research assistant)
Participant: Royce Reyes
Person Months Worked: 6.00 **Funding Support:**
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National Academy Member: N

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Participant: Kanis Bootsita
Person Months Worked: 1.00 **Funding Support:**
Project Contribution:
National Academy Member: N

Participant Type: Undergraduate Student
Participant: Nicolas Mabilleau
Person Months Worked: 1.00 **Funding Support:**
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Article Title: Nanoscale dislocation shear loops at static equilibrium and finite temperature
Authors: Khanh Dang, Laurent Capolungo, Douglas E Spearot
Keywords: atomistic simulations, discrete dislocation dynamics simulations, dislocation shear loops, aluminum
Abstract: Atomistic simulations are used to determine the resolved shear stress necessary for equilibrium and the resulting geometry of nanoscale dislocation shear loops in Al. Dislocation loops with different sizes and shapes are created via superposition of elemental triangular dislocation displacement fields in the presence of an externally imposed shear stress. First, a bisection algorithm is developed to determine systematically the resolved shear stress necessary for equilibrium at 0 K. This approach allows for the identification of dislocation core structure and a correlation between dislocation loop size, shape and the computed shear stress for equilibrium. It is found, in agreement with predictions made by Scattergood and Bacon, that the equilibrium shape of a dislocation loop becomes more circular with increasing loop size. Second, the bisection algorithm is extended to study the influence of temperature on the resolved shear stress necessary for stability. An approach is presented to
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Article Title: Pressure Dependence of the Peierls Stress in Aluminum
Authors: Khanh Dang, Douglas Spearot
Keywords: Atomistic simulations, Peierls stress, interatomic potentials
Abstract: The effect of pressure applied normal to the {111} slip plane on the Peierls stress in Al is studied via atomistic simulations. Edge, screw, 30o, and 60o straight dislocations are created using the Volterra displacement fields for isotropic elasticity. For each dislocation character angle, the Peierls stress is calculated based on the change in the internal energy, which is an invariant measure of the dislocation driving force. It is found that the Peierls stress for dislocations under zero pressure is in general agreement with previous results. For the screw and 60o dislocations, the Peierls stress versus pressure relationship has maximum values associated with stacking fault widths that are multiples of the Peierls period. For the edge dislocation, the Peierls stress decreases with increasing pressure from tension to compression. Compared to the Mendelev potential, the Peierls stress calculated from the Mishin potential is more sensitive to changes in pressure.
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Article Title: Mobility of dislocations in Aluminum: Faceting and asymmetry during nanoscale dislocation shear loop expansion
Authors: Khanh Dang, Darshan Bamney, Kanis Bootsita, Laurent Capolungo, Douglas E. Spearot
Keywords: Dislocation mobility, Dislocation loops, Molecular dynamics, Dislocation dynamics
Abstract: Dislocation loop expansion in Al is studied with a hierarchical multiscale approach via atomistic and discrete dislocation dynamics simulations. First, mobility laws for straight screw, 30°, 60°, and edge dislocations are calculated using molecular dynamics (MD) simulations. Each atomistic mobility law is described by an empirical piecewise function with a character angle dependent power law exponent to capture the nonlinear damping regime. For the dislocation velocity range considered in this work, the mobilities of screw and 60° dislocations are lower than edge and 30° dislocations. The mobilities of mixed dislocations, such as 30° and 60°, are found to depend on the character of the leading Shockley partial. Second, MD simulations of dislocation loop expansion under a constant external Schmid stress are performed. The expanded dislocation loop is found to facet in the 60° and screw segments due to low mobilities. The dislocation loop is also found to have reflection asymmetry.
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Title: Atomistic Simulations of Dislocation Properties and the Role of Stress State in Aluminum
Authors: Khanh Quoc Dang
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Title: Towards Physicall Representative Dislocation Dynamics Models for Polycrystalline Plasticity
Authors: Darshan Bamney
Acknowledged Federal Support: **Y**

Partners

,

Dr. Laurent CapolungoLos Alamos National LaboratoryDr. Capolungo's team is the original authors of the DDD code

I certify that the information in the report is complete and accurate:
Signature: Douglas Edward Spearot
Signature Date: 8/3/21 8:36AM

Equations

$$\tau_{friction} = \tau_{sd,T} - \frac{G_T}{G_{400K}} \tau_{sd,400K} \tag{1}$$

$$\sigma = \begin{cases} B\upsilon & if\ \upsilon \le \upsilon_o \\ B\upsilon + D\left(\upsilon - \upsilon_o\right)^a & if\ \upsilon > \upsilon_o \end{cases} . \tag{2}$$

Figures

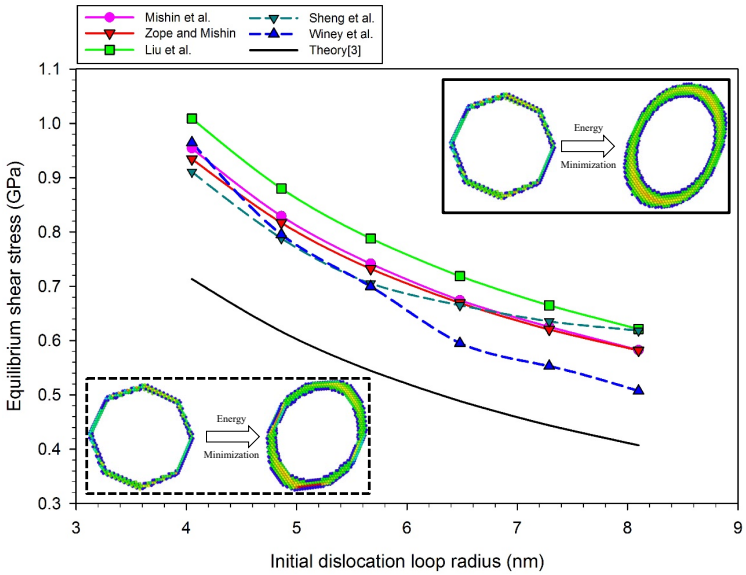

Figure 1. Equilibrium resolved shear stress for different loop radii and different Al EAM potentials. Solid curves and box outline indicate potentials that provide successful relaxation. Dashed curves and box outline indicate potentials that provide unsuccessful relaxation. Only atoms with centrosymmetry values higher than 2.0 $Å^2$ are shown.

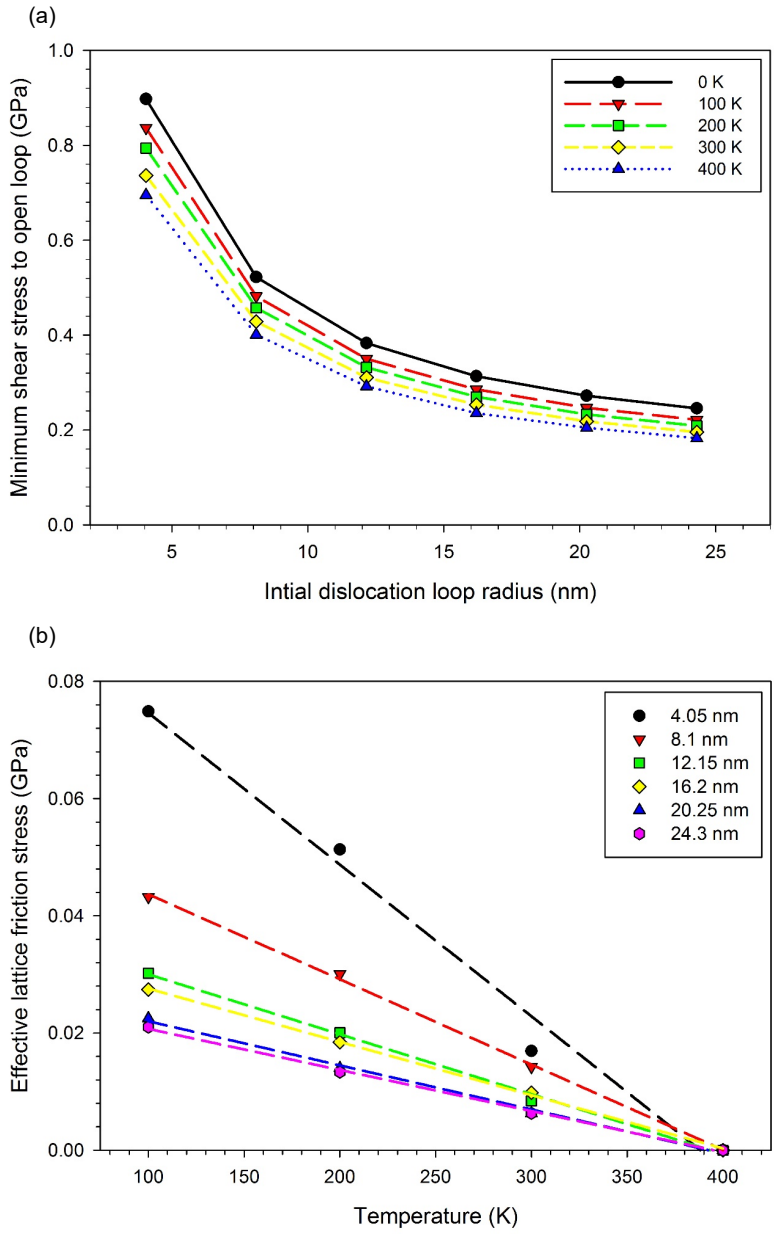

Figure 2. (a) Minimum shear stress in the Burgers vector direction to open a dislocation loop and (b) effective lattice friction stress for different initial dislocation loop radii and temperatures.

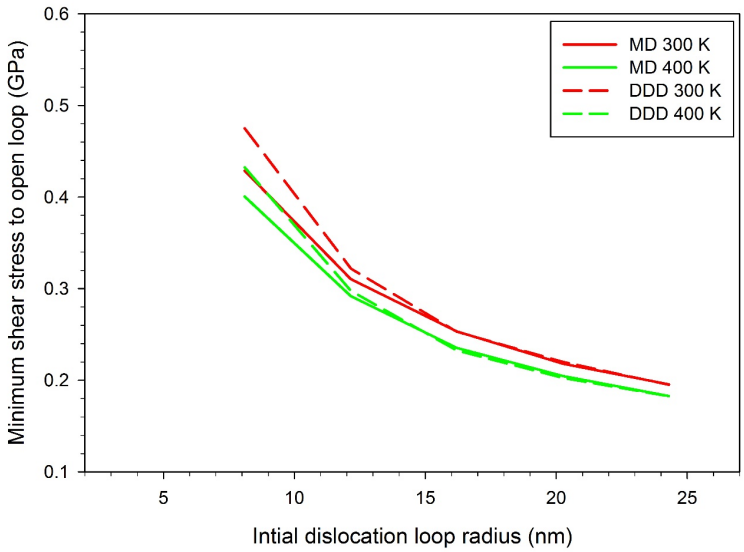

Figure 3. Comparison between MD and DDD data at 300 and 400 K. The core width parameter in DDD is tuned to match the MD data using the temperature dependence of the elastic moduli and friction stress extracted from MD.

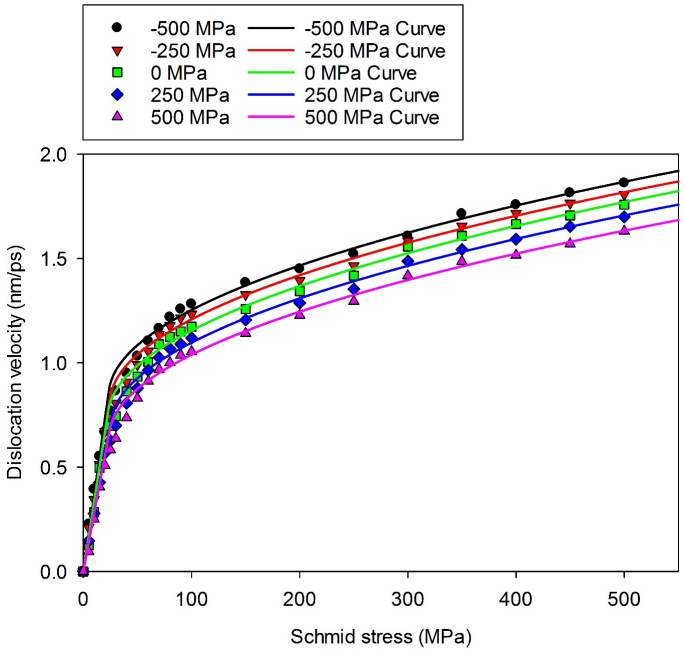

Figure 4. Mobility data and curves (Eq. (2)) for screw dislocations under different pressures normal to the (111) slip plane and Schmid stresses.

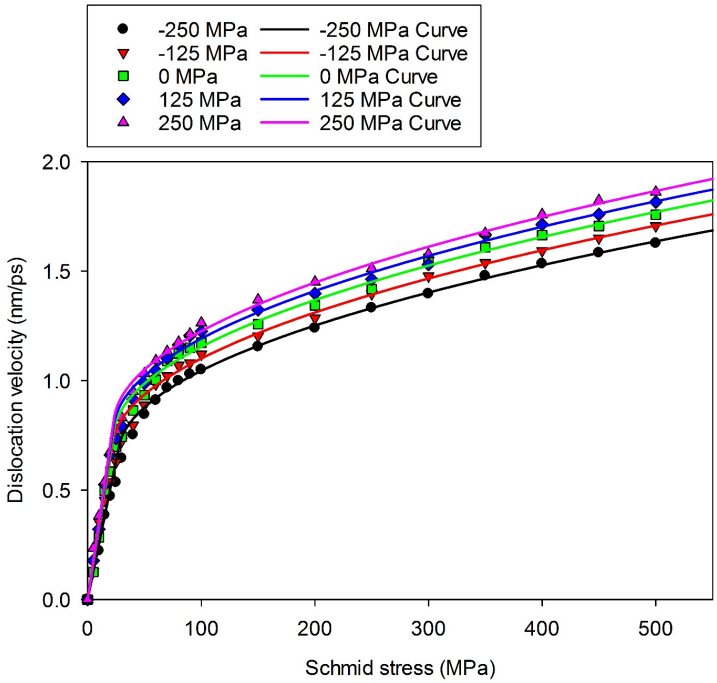

Figure 5. Mobility data and curves (Eq. (2)) for screw dislocations under different Escaig and Schmid stresses.

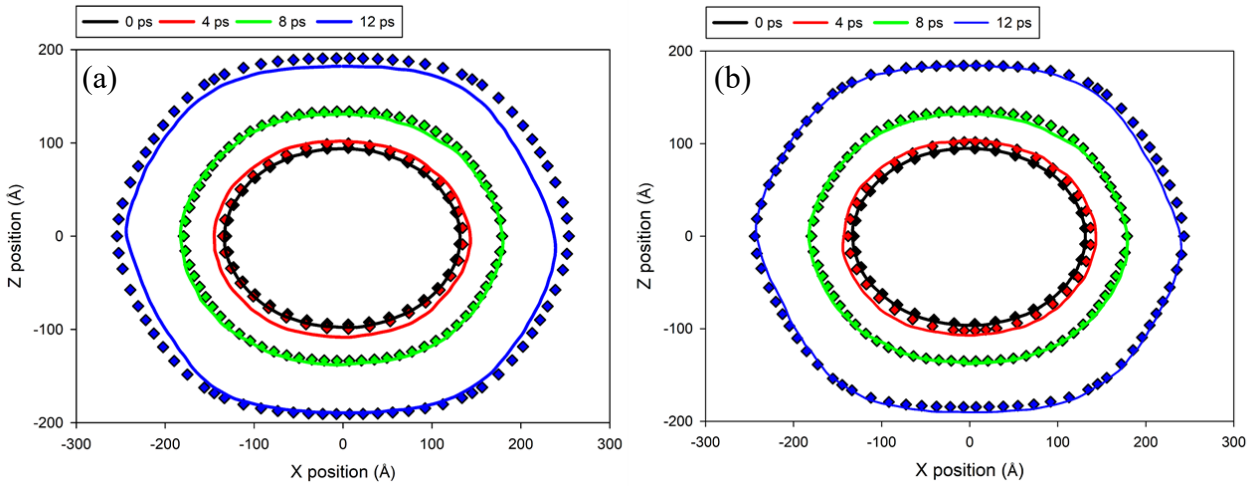

Figure 6. Comparison of the time evolution (0, 4, 8, and 12 ps) of the dislocation loop geometry under a Schmid stress of 380 MPa and (a) τ_e = 250 MPa, and (b) σ_n = 500 MPa. The solid lines represent MD data (average of partial dislocation core positions) and the filled diamond markers indicate DDD data. Strong agreement between MD and DDD data is observed validating the implementation scheme for mixed dislocations.

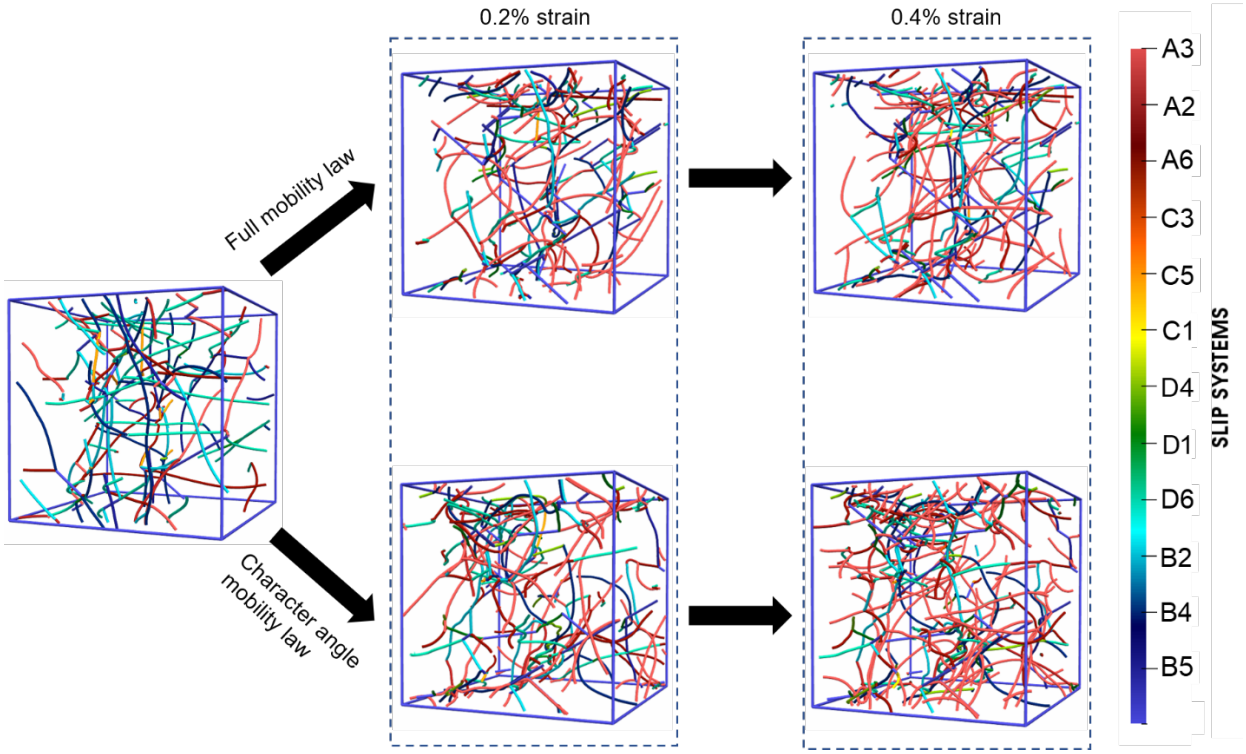

Figure 7. Comparison of the dislocation microstructures developed after 0.2% and 0.4% axial strains along the [123] direction for the two prescribed mobility laws starting from the same initial network. The slip systems are indicated using the Schmid and Boas notation.

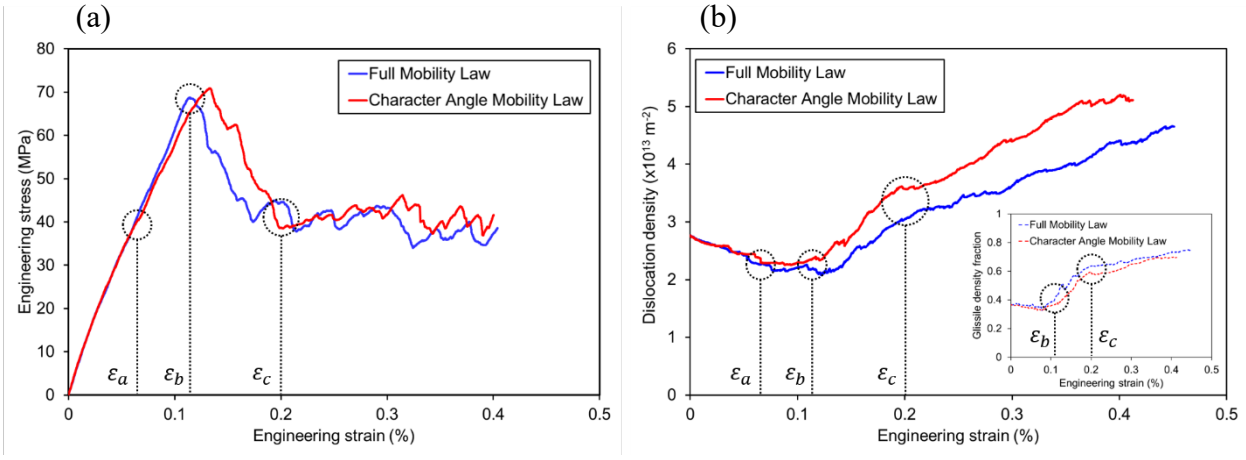

Figure 8. (a) Comparison of the engineering stress-strain relationships and (b) the evolution of the total dislocation density using two different mobility law forms. The ratio of the density on the active slip systems to the total dislocation density is also shown in the inset of (b).

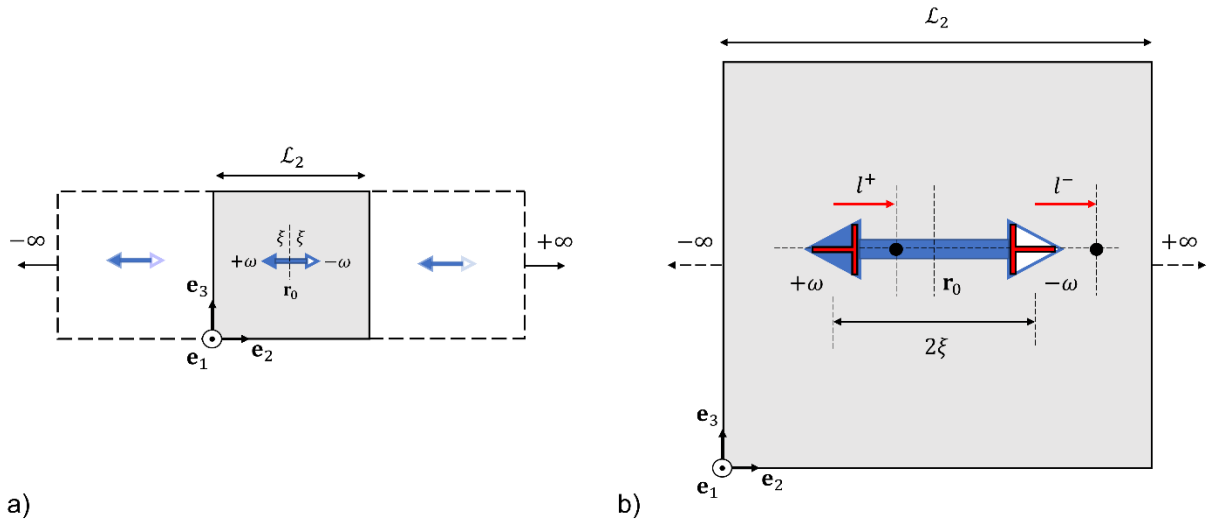

Figure 9. (a) Simulation box showing an infinitely long wedge disclination dipole (WDD) of strength $\pm\omega$ and arm length 2ξ aligned with the $\mathbf{e_1}$-axis. The image cells for the analytical summation of the WDD stress fields along the $\mathbf{e_2}$-direction for the periodic models are shown via dashed boxes. (b) Simulation cell showing an infinitely long WDD with rotation axis shifts of l^+ and l^-. The positions of the new rotation axes are indicated by •. The corresponding infinitely long edge dislocations of Burgers magnitude $b^+ = -\omega l^+$ and $b^- = \omega l^-$, resulting from the rotation axis shifts, are also shown.

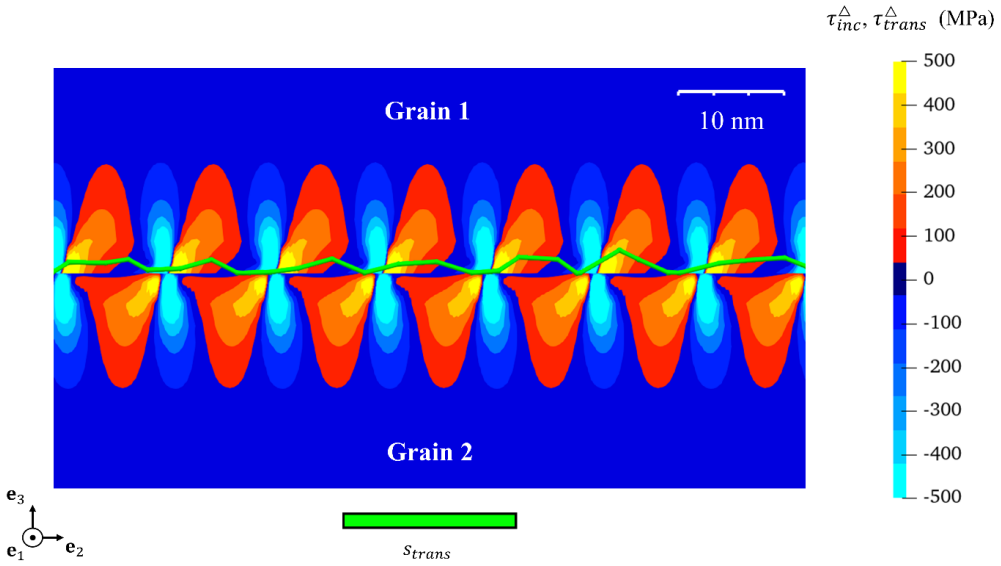

Figure 10. Transmission nuclei formed on the $s_{trans} = \frac{1}{2}[\bar{1}01]_1(111)_1$ slip system in the outgoing grain (grain 1) for the equilibrium $\Sigma 627$ grain boundary simulation at $\tau^{ext} \approx 500\,MPa$. The transmission nuclei (green) are superimposed on maps of the GB shear stresses resolved on the incoming slip system in grain 2 ($\tau^{\triangle}_{inc}$) and on the outgoing slip system in grain 1 ($\tau^{\triangle}_{trans}$). Only the dislocations on the transmission slip system are shown for clarity.

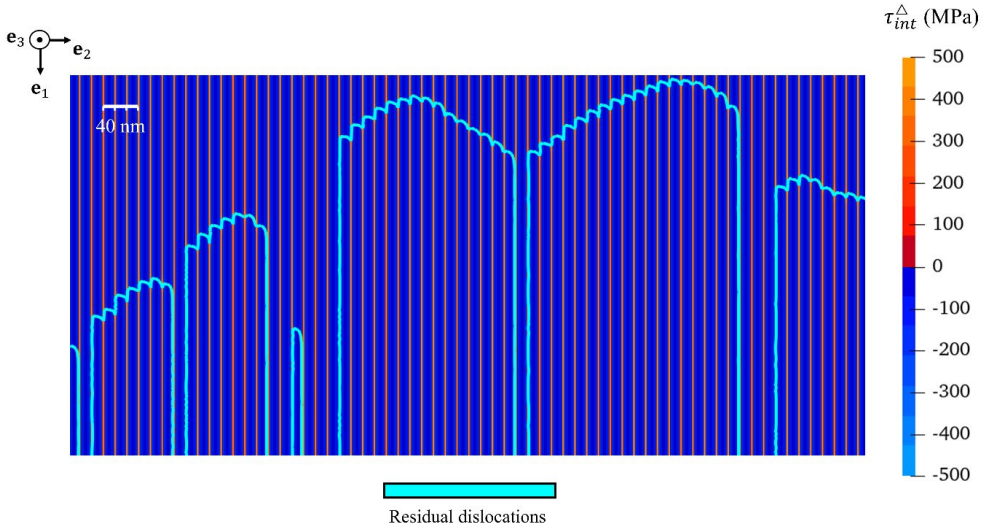

Figure 11. Residual dislocation configuration on the $(\bar{7}\,7\,34)_2$ GB plane for the equilibrium $\Sigma 627$ grain boundary simulation at $\tau^{ext} \approx 500\,MPa$. The residual (cyan) dislocation lines are superimposed on the map of the GB shear stress resolved on the interface ($\tau^{\triangle}_{int}$). The scale bar is rescaled to highlight the positions of the wedge disclination dipole cores, which are indicated by the fine lines in the $\tau^{\triangle}_{int}$ map.

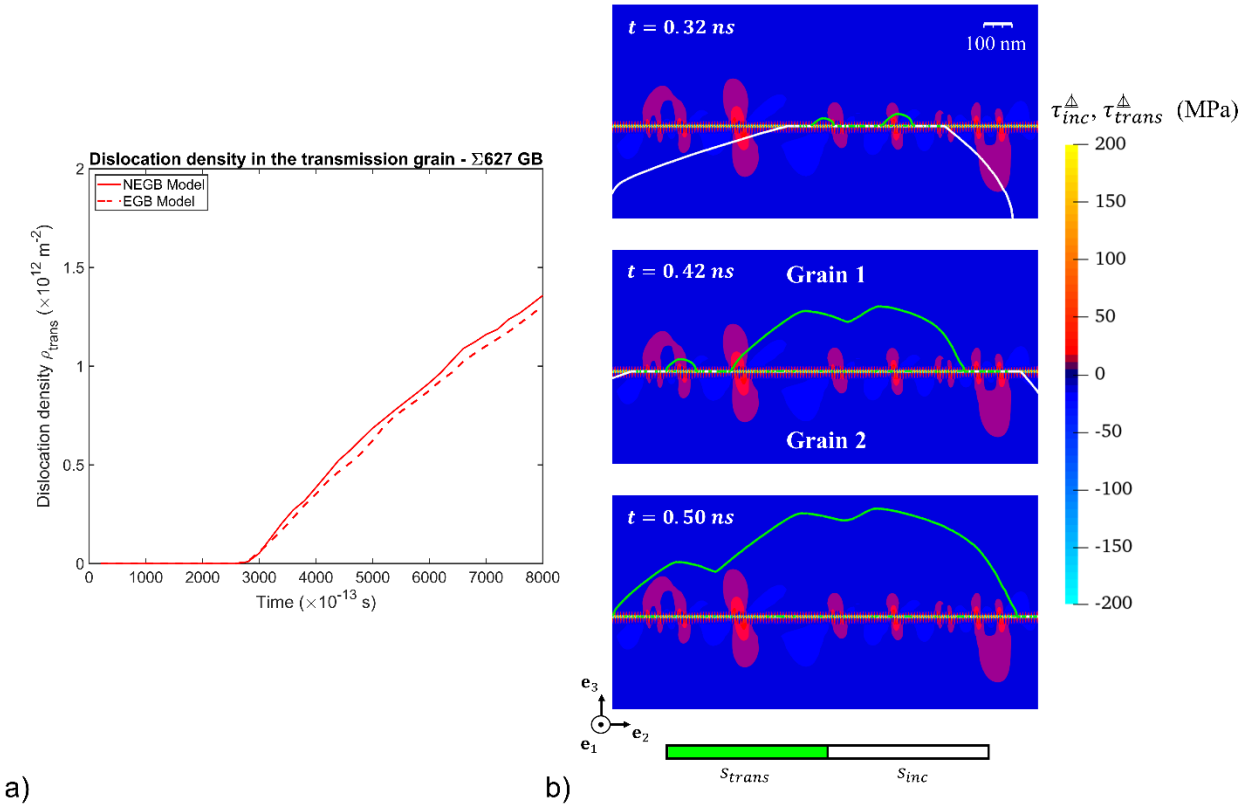

Figure 12. (a) Comparison of dislocation density ρ_{trans} evolution in grain 1 (transmission grain) for the equilibrium and non-equilibrium Σ627 GBs at $\tau^{ext} \approx 500\,MPa$. (b) Snapshots of the dislocation transmission events occurring during the NEGB simulation for the Σ627 GB. The dislocation lines on s_{inc} (white) and s_{trans} (green) are superimposed on maps of the GB shear stresses resolved on the respective slip systems in grain 2 ($\tau^{\triangle}_{inc}$) and grain 1 ($\tau^{\triangle}_{trans}$). The scale bar is rescaled to highlight the long-range stresses induced by the complexes of wedge disclination dipoles and extrinsic dislocations at the GB

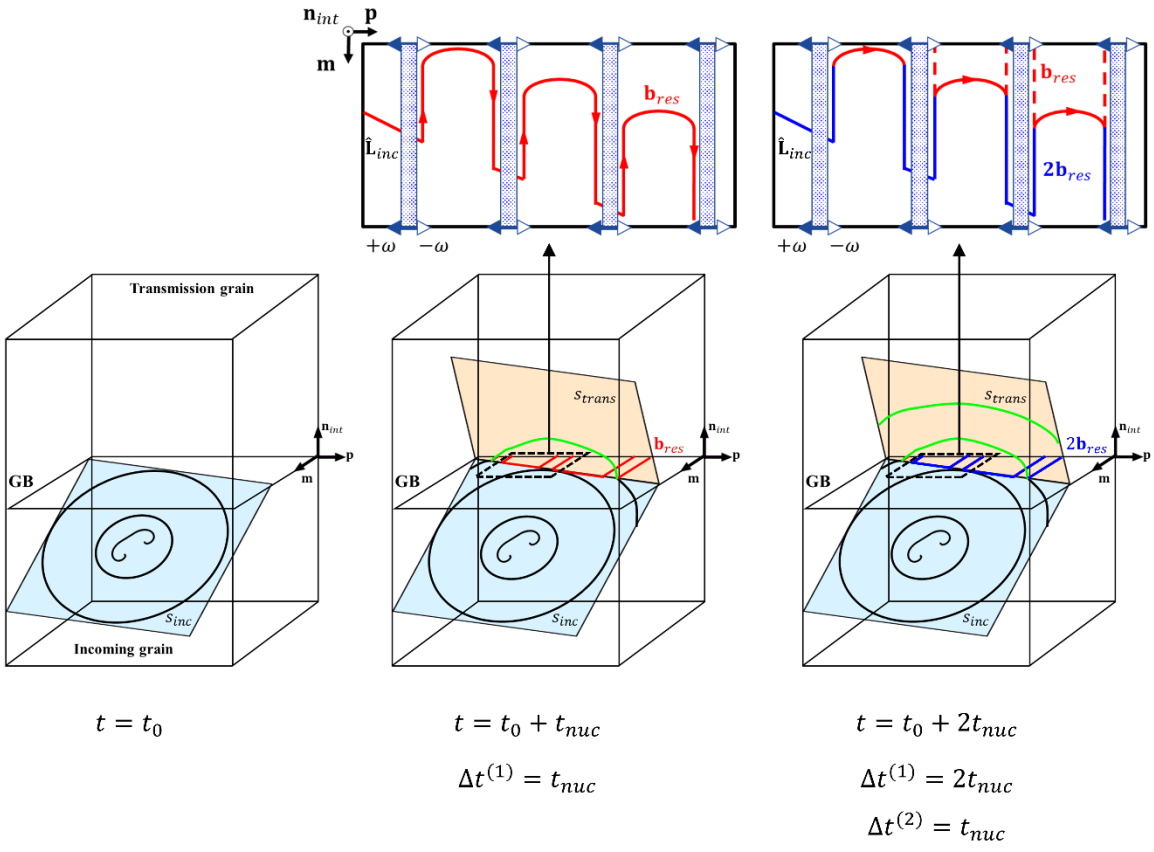

Figure 13. Schematic depicting the formation and evolution of NEGBs by dislocation transmission. (a) The Frank-Read source on the incoming slip system s_{inc} nucleates elliptical dislocation loops that expand in the incoming grain. At time $t = t_0$, the first dislocation loop impinges on the GB. (b) At time $t = t_0 + t_{nuc}$, the second loop nucleated from the Frank-Read source arrives at the GB. During the time interval $\Delta t^{(1)} = t_{nuc}$, the initial loop coherently transmits through the GB onto s_{trans}, depositing residual dislocations with Burgers $\mathbf{b}_{res}$ on the GB plane. The residual dislocations propagate on the GB plane via a threading process depositing straight dislocations in the vicinity of the disclinations ($\pm\omega$) as illustrated in the magnified inset. (c) A third loop reaches the GB at time $t = t_0 + 2t_{nuc}$. During the time interval $\Delta t^{(2)} = t_{nuc}$, the second loop transmits through the GB and the propagating residual dislocations interact with the previously deposited residuals, resulting in dislocations with Burgers $2\mathbf{b}_{res}$ on the GB plane, as shown in the inset. The first loop has expanded further along the slip trace during this time interval, depositing additional residual dislocation content. The misorientation axis and GB normal are indicated by $\mathbf{m}$ and $\mathbf{n}_{int}$, respectively.

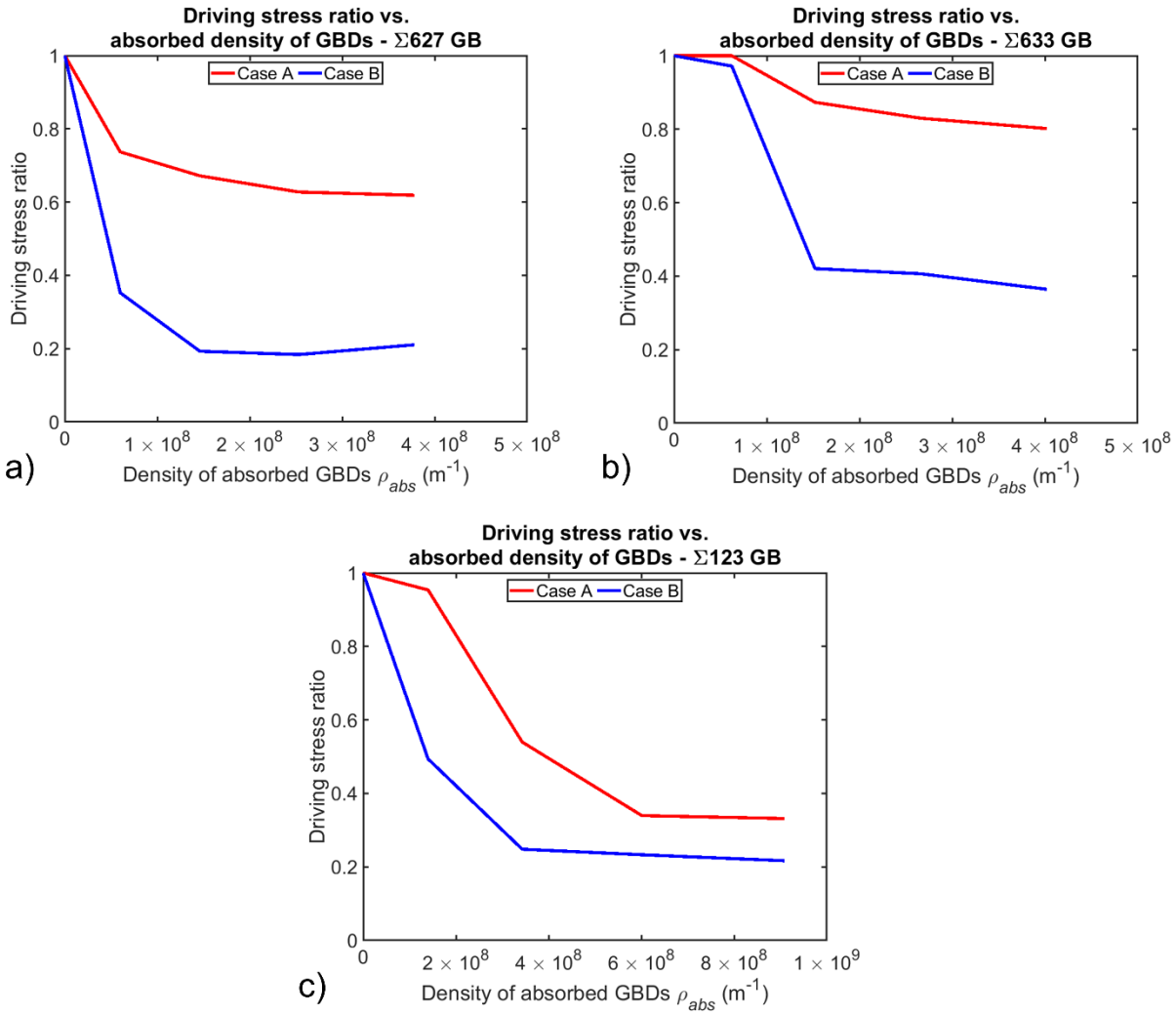

Figure 14. Driving stress ratio versus density of absorbed extrinsic grain boundary dislocation (ρ_{abs}) for the (a) Σ627, (b) Σ633, and (c) Σ123 GBs. The curves are shown for transmission through both Case A and Case B NEGBs (two different prior transmission event types). Note, the ρ_{abs} axis is different for the Σ123 boundary compared to the other two GBs due to differences in the areal density of wedge disclination dipoles at the GB.

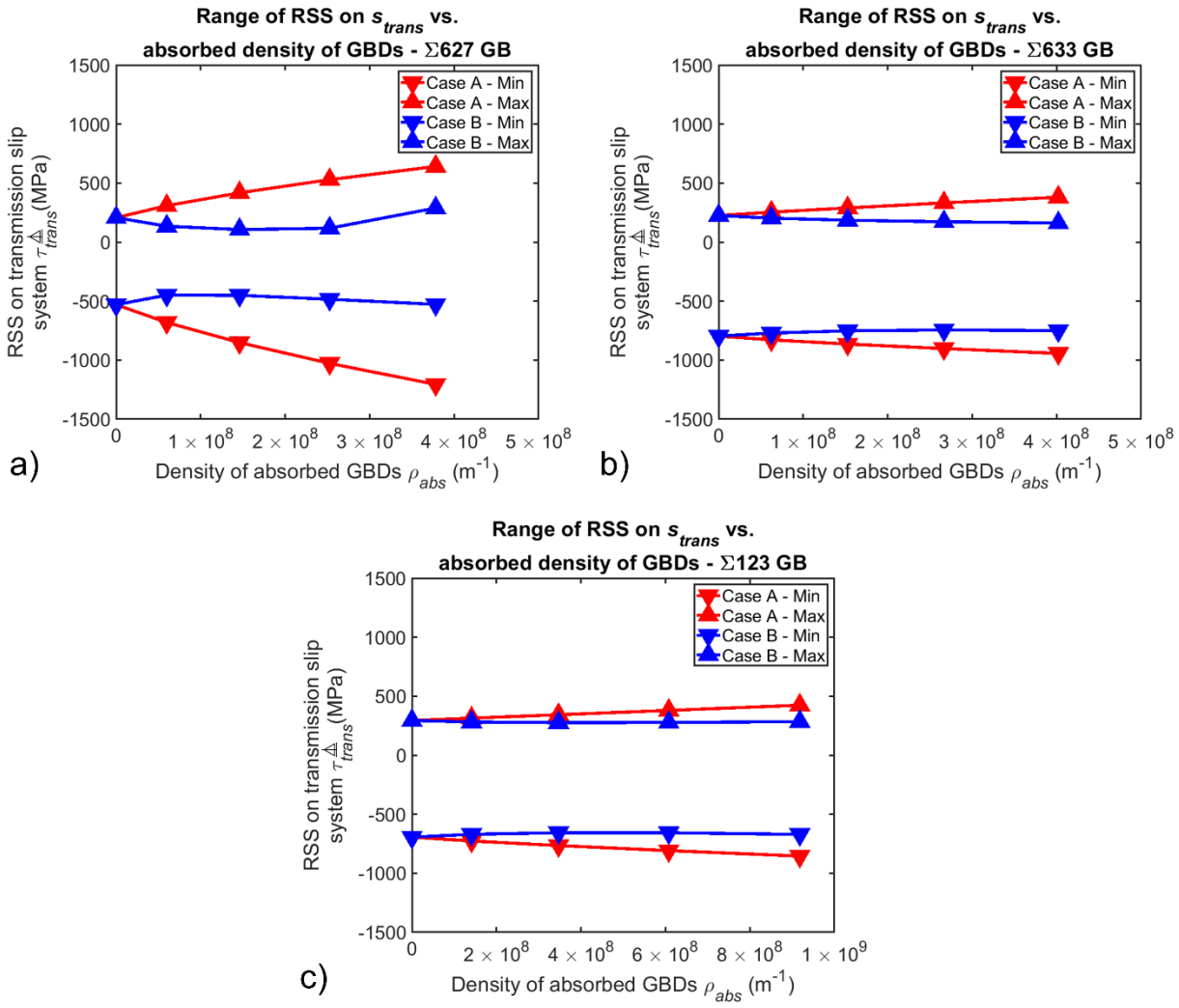

Figure 15. Minimum and maximum values of the resolved shear stresses on s_{trans} due to the GB ($\tau^{\triangleq}_{trans}$) versus density of absorbed GBDs ρ_{abs} for the (a) Σ627, (b) Σ633, and (c) Σ123 GBs. The curves are shown for both Case A and Case B nonequilibrium grain boundaries for each misorientation. The values of $\tau^{\triangleq}_{trans}$ are measured in the region with maximum absorbed GBD content and at a distance of 1 nm from the GB plane in the outgoing grain in all cases. This data shows that the resolved shear stress on the outgoing slip system is not solely responsible for the reduction in critical shear stress for transmission in Fig. 14.

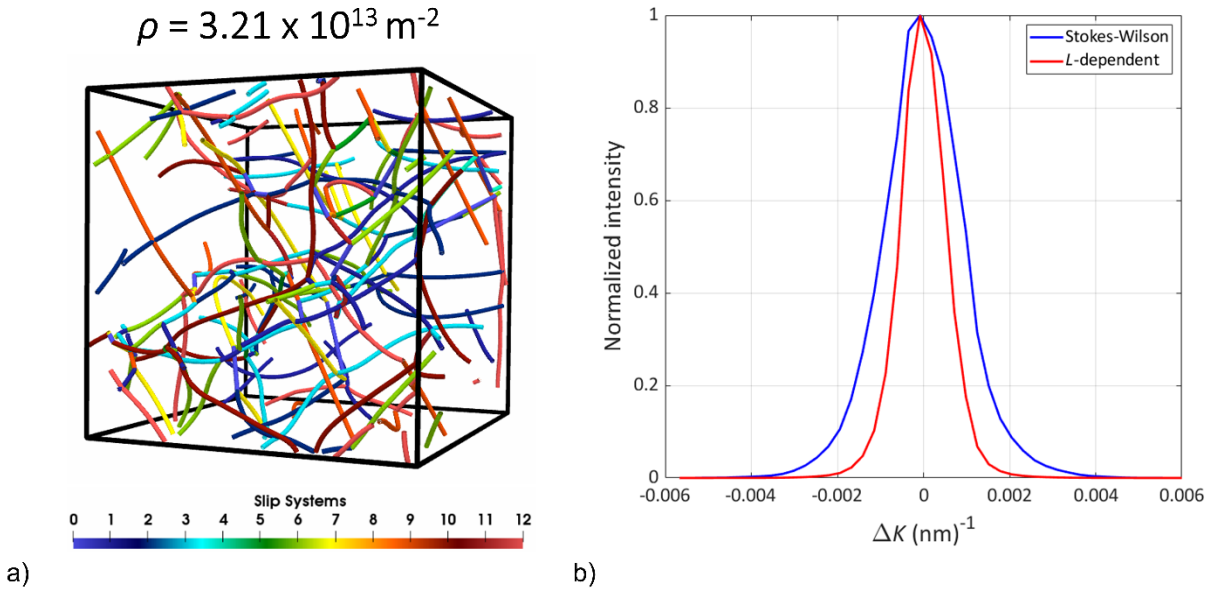

Figure 16. (a) Equilibrated dislocation configuration obtained from a DDD-FFT simulation with grid size of $N_{FFT} = 64 \times 64 \times 64$ having average dislocation density $\rho = 3.21 \times 10^{13}\ m^{-2}$ and (b) comparison of the normalized intensity profiles for $\mathbf{K} = [111]$.

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