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Original Article

Ensemble Kalman Filter–based Multi-Parameter Identification of Dislocation Mobility in Discrete Dislocation Dynamics

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Abstract - *To enhance the predictive ability of Discrete Dislocation Dynamics (DDD) simulations applied to study plastic deformation and microstructural evolution in crystalline materials, it is necessary to identify the dislocation mobility parameters accurately. This paper introduces an inverse modeling algorithm, which is based on the EnKF, for the joint estimation of screw, edge, and climb mobility parameters based on the observations of the trajectory of the dislocation nodes. The proposed solution incorporates both physics-based DDD forward model and sequential data assimilation by means of an augmented-state formulation that encompasses and defines both dislocation node coordinates and unknown mobility parameters. The forward simulations of DDD with known reference parameters and controlled measurement noise are used to generate synthetic observation data in order to allow the systematic validation of the framework. The convergence of parameters, the reconstruction accuracy, dependence on observation noise, dependence on ensemble size, and uncertainty quantification are some of the performance measures of the proposed method. Findings show that the EnKF system can effectively reconstruct the target mobility parameters with relative errors less than 1 percent and, at the same time, enhance the reconstruction of the changing dislocation structures. The uncertainty analysis also shows that there are no significant changes in the estimates of the parameters with close confidence intervals in the conditions of the synthetic benchmarks considered. The suggested framework offers an effective and uncertainty-sensitive methodology to identify mobility parameters and illustrates the promise of integrating physics-based methods to compute dislocation dynamics into ensemble data assimilation algorithms to make inferences about materials through computational methods.*

Keywords - *Discrete Dislocation Dynamics, Ensemble Kalman Filter, Mobility Parameter Estimation, Data Assimilation, Uncertainty quantification.*

1. Introduction

Dislocations, motions and interaction are the essential factors that control plastic deformation of crystalline materials. The movement of dislocations dictates the rate of dislocations to the applied stresses, hence has a direct effect on the mechanical behaviour, including yielding, strain hardening and creep. Mobility of dislocations is thus fundamental to understanding and proper modelling of the behaviour of microstructural evolution and mechanical properties of structural materials [1, 2].

Discrete Dislocation Dynamics (DDD) has become a promising computational tool to investigate the dynamics of dislocation networks of crystalline materials. Existing DDD simulations represent dislocations as line defects, which are discretized into segments, and respond to elastic stress fields and external loading conditions [1, 4, 5]. Such simulations enable researchers to model complicated processes and, therefore, dislocation multiplication, interaction, annihilation, and junction formation and understand the mesoscale processes that control plastic deformation [2, 4]. Developing dislocation mobility and the effects of dislocation character on movement have been extensively investigated in mesoscale and atomistic simulations, which have underscored the significance of mobility laws in faithful simulation of crystal plasticity behaviour [3, 7, 14].

Although these are the benefits, DDD simulations are based on a number of mobility parameters that explain the correlation between forces applied and the dislocation velocity. Estimation of these parameters is an uphill task. Traditional methods of mobility parameters estimation are usually based on the correspondence of the output of simulations to experimental data or atomistic simulation results, although they usually aim at the single-parameter estimation and might be computationally intensive [15, 19]. In addition, such methods might be inadequate to fully consider uncertainty in measurements or disparity in underlying physical operations that control dislocation movement [13].

Methods of data assimilation offer an alternative approach to the estimation of parameters, as they combine observations and numerical calculation. Ensemble Kalman Filter (EnKF) is one of these methods, and has been broadly used in meteorology, ocean modelling and nonlinear dynamical systems to estimate both system states and parameters at the same time [6, 9, 11]. The EnKF has the following advantages: computational efficiency, ability to propagate moderately nonlinear systems and the potential to update both model states and unknown parameters in sequential assimilation [6, 8, 18]. These characteristics are what draw the EnKF especially to the coupled state/parameter estimation problems.

Most recently, computational materials science and multiscale modelling have started to be studied using data assimilation techniques and Bayesian inverse modelling [10, 20]. Such methods enable model parameters to be estimated by using the data of observations whilst taking into consideration the uncertainty of model prediction, as well as of measurements. Ensemble-based assimilation methods have also been used to estimate the constitutive parameters of simulating crystal plasticity and other multiscale materials [16]. Besides this, data-driven and inverse modelling methods have been explored to predict microstructure evolution and discover material parameters on both synthetic and experimental datasets [17].

Nevertheless, the use of sequential dislocation simulations at the microstructure scale with the application of sequential data assimilation techniques is still relatively low. Specifically, algorithms that can estimate various dislocation mobility parameters at the same time are not yet well-developed in a discrete dislocation dynamics model. Although recent work in inverse modelling, Bayesian calibration, and data assimilation of computational materials science has been done, a systematic framework of jointly estimating multiple dislocation mobility parameters directly on a discrete dislocation dynamics scale has not yet been adequately developed [12]. Specifically, little has been done as to the joint estimation of screw, edge and climb mobility parameters based on sequential assimilation of dislocation node paths.

Most of the existing calibration methods are based on manual tuning, optimization-based tuning or atomistic reference data, even though DDD simulations have been extensively used to investigate the evolution of dislocations. The methods usually concentrate on the estimation of just one parameter and do not explicitly update the dislocation conditions as well as the mobility parameters during the simulation. Specifically, the sequential data assimilation of screw, edge, and climb mobility parameters at the DDD scale has not been developed properly yet. This discrepancy inspires the current EnKF-based multi-parameter inverse modeling model. This deficit has inspired the current design, which integrates physics-founded DDD forward model with an ensemble data assimilation design to identify multiple parameters. This study aims to establish a multi-parameter inverse modelling structure in estimating the dislocation mobility parameters based on ensemble data assimilation. The given framework involves the DDD simulation in combination with the Ensemble Kalman Filter and analyses the synthetic observation data to compare the performance of the approach.

This paper constructs a data-assimilative inverse model that is used in determining dislocation mobility parameters in discrete dislocation dynamics simulations. The principal contributions are as follows. A formulation is first presented, which is an augmented-state formulation, in which both dislocation node coordinates and mobility parameters are updated at the same time. Second, a synthetic observation generation procedure is characterised in order to permit controlled validation of the estimation structure. Third, the Ensemble Kalman filter is combined with the DDD solver to correct the microstructural state and the unknown mobility parameters successively. Lastly, parameter convergence, reconstruction accuracy, sensitivity to observation noise and ensemble size are also tested with the help of numerical experiments.

Table 1. Comparison of the proposed work with existing approaches

Approach	DDD-based	Multi-parameter mobility estimation	Sequential data assimilation	Explicit uncertainty handling
Conventional DDD calibration	Yes	Limited	No	Limited
Atomistic mobility fitting	No	Partial	No	Limited
Bayesian materials calibration	Partial	Yes	No	Yes
Proposed EnKF–DDD framework	Yes	Yes	Yes	Yes

Conventional DDD calibration schemes, as summarized in Table 1, are mainly based on parameter tuning and do not do sequential state-parameter updating, whereas atomistic fitting schemes are mainly based on the derivation of mobility laws, but not dynamic assimilation. Bayesian calibration methods are able to give quantification of uncertainty, but tend not to be coupled directly to discrete dislocation dynamics to perform sequential multi-parameter learning. In comparison, EnKF -DDD proposed framework integrates physics-based simulation of the DDD and augmented-state Ensemble Kalman filtering, allowing simultaneous estimation of screw, edge, and climb mobility parameters along with the constant update of the coordinates of dislocation nodes. It is a combined ability that makes up the main originality of the given work.

2. Methodology

2.1. Physics-based Discrete Dislocation Dynamics Model

Physical dynamics of dislocations are modeled with a Discrete Dislocation Dynamics (DDD) model, where dislocations are modeled as a line defect discretized into nodes linked by straight segments. The segments are defined with their Burgers vector and local line direction, and the screw, edge and mixed dislocation character could be represented. The flow of every node is estimated by the equilibrium of forces on the dislocation segments, which will be self-forces, stresses on the neighboring segments, and external forces. The force on a piece of dislocation is determined by the Peach-Koehler relation.

$$F = (\sigma \cdot b) \times \xi$$

In which σ denotes the stress used, bis the Burgers, and ξ is the unit vector indicating the local direction of the line of dislocation segment. In this case, F represents the overall force that exists on the dislocation segment because of the resultant response of the applied stress field and the dislocation line. In the situation of overdamped dynamics, the speed of a dislocation node is proportional to the exerted force.

$$v = MF$$

M is the coefficient of dislocation mobility, and v is the nodal velocity. In real materials, mobility is determined by the nature of the dislocation and the mechanism of deformation. Thus, a multi-parameter mobility model is taken where screw, edge, and climb motions are modelled in terms of individual mobility parameters.

$$\theta = [M_s, M_e, M_c]$$

where M_s, M_e, and $M_c$are the mobility coefficients of screw, edge, and climb -dislocation motion, respectively. The model can be parameterized to differentiate between various kinetic reactions of separate dislocation characters. The dynamic dislocation node movement is calculated using explicit time integration.

$$x_{t+\Delta t} = x_t + v_t \Delta t$$

where $x_t$represents nodal position at time t, v_t is nodal velocity, and Δt represents a time step in the simulation. This time integration method permits the development of a dislocation network to be modelled with the given loading conditions. The node trajectories resulting from the situation of the evolving dislocation and forms the physical state variables in the next inverse modelling. The DDD model is utilised in the current research as a controlled forward simulator in assessing the proposed parameter estimation framework. The formulation is aimed at modelling the kinematic evolution of the discretized dislocation nodes under prescribed loading and mobility laws as opposed to a material-specific high-fidelity calibration of constitutive laws. Based on this, emphasis is made on developing a steady forward- inverse workflow and determining the recoverability of mobility parameters in synthetic observations.

The general formulation of dislocation geometry, forces and relations of mobility in the DDD framework is presented in Figure 1, which depicts the discrete dislocation segments, applied stress direction and force- velocity relation defining node movement.

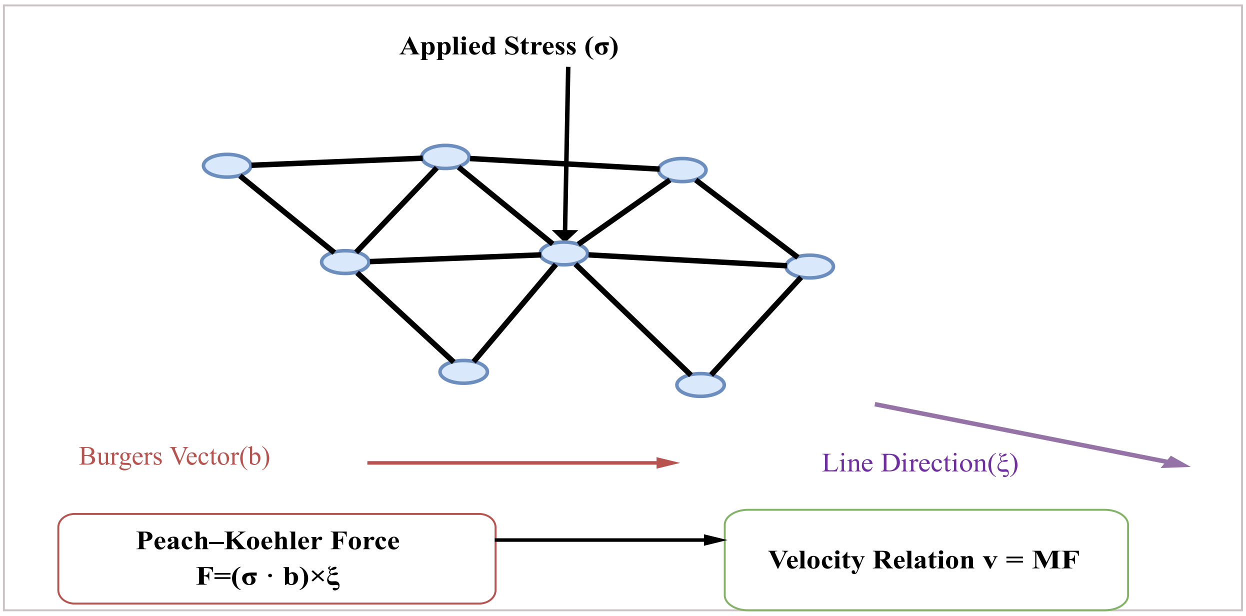

Fig. 1 Schematic representation of the discrete dislocation dynamics model showing node discretization, Burgers vector orientation, and force-driven dislocation motion

2.2. Synthetic Observation Data Generation

In order to test the parameter estimation framework under controlled circumstances, the synthetic observation data are produced by the forward simulation of DDD with known mobility parameters. With the use of synthetic observations, the inverse modelling approach can be systematically validated since the actual values of the parameters are known in advance. The forward simulation generates time-dependent dislocation configurations in the form of node coordinates. It can be observed that the observation vector at time t is defined as

$$y_t = [x_1, y_1, z_1, \dots, x_N, y_N, z_N]^T$$

where N represents the count of dislocation nodes that have been discretized, in order to have the measurement uncertainties as in an experiment, Gaussian noise is superimposed on the observations.

$$y_t^{obs} = y_t + \epsilon$$

where the noise term follows a normal distribution

$$\epsilon \sim N(0, R)$$

R is the covariance of the observation. This noise takes into consideration measurement errors that might occur in experimental imaging methods like transmission electron microscopy. The present study is based on the assumption of additive Gaussian noise, which is a first-order model of measurement uncertainty. In real-world experimental measurements, noise can be non-Gaussian, correlated or due to node tracking incompleteness. These effects may affect the quality of parameter estimation, and must be addressed in future research with more realistic observation models and effective filtering mechanisms. The synthetic observation generation process is composed of the following steps:

1. Define material parameters and simulation domain.
2. Perform forward DDD simulation using known mobility parameters
3. Extract dislocation node coordinates at selected time intervals
4. Add Gaussian noise to simulate measurement uncertainty

Such a workflow generates a dataset that is a representation of quantifiable dislocation structures, which can be incorporated into the inverse modelling framework. The entire scheme of creating synthetic observations involves forward simulations that generate dislocation paths and transforming them into noisy observation data to be assimilated, which can be seen in Figure 2.

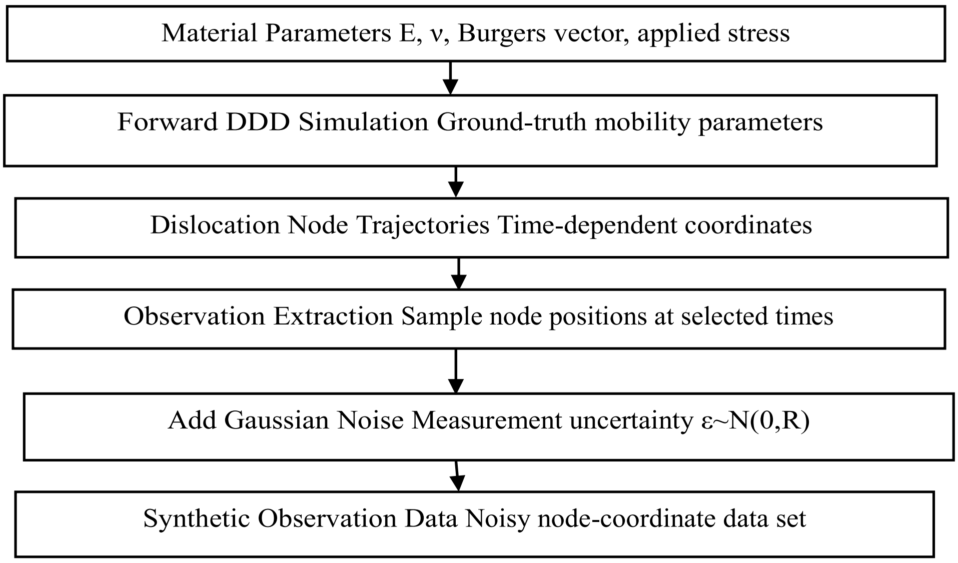

Fig. 2 Workflow for synthetic observation generation from forward DDD simulations, including extraction of node coordinates and addition of measurement noise

Table2. Simulation parameters used in numerical experiments

Parameter	**Value**
Crystal structure	BCC
Young's modulus	170 GPa
Poisson ratio	0.33
Burgers vector magnitude	0.255 nm
Applied shear stress	0.5 GPa
Ensemble size	30
Observation noise standard deviation	0.01
Simulation time step	Δt
Observation interval	Δt_{obs}

Table 2, which contains the material properties of the considered study, loading conditions, ensemble size, and observation noise level are the key simulation parameter to be used to generate synthetic observation data and carry out the experiments of assimilation.

2.3. Ensemble Kalman Filter-based Inverse Modeling Framework

A data assimilation framework using the Ensemble Kalman Filter (EnKF) is used to estimate the dislocation mobility parameters using the synthetic observation data.

The EnKF involves a combination of both the observational data and numerical simulations to update both the state of the system and the unknown parameters. The system state vector is formulated to comprise dislocation geometry as well as mobility parameters.

$$X = [x, \theta]$$

where x is the coordinates of dislocation nodes, and θ is the set of mobility parameters to estimate. In the current experiment, the mobility parameter vector is as given below:

$$\theta = [M_s, M_e, M_c]$$

where M_s, M_e, and $M_c$are the screw, edge and climb mobility parameters, respectively. In the sequential assimilation procedure, the augmented state vector at time t is expressed as.

$$S_t = \begin{bmatrix} X_t \\ \theta \end{bmatrix}$$

where $X_t$was defined as the dislocation node coordinates at time $t$and θ was the unknown mobility parameter. A set of system states is provided as an expression of uncertainty in the initial parameter estimates.

$$S_t^{(k)} = [X_t^{(k)}, \theta^{(k)}]$$

where $k = 1,2, \dots, N_e$, are the members of the ensemble, and $N_e$is the size of the ensemble. In the prediction stage, all the ensemble members are independently evolved with the forward DDD simulation.

$$S_{t+1}^{(k)} = F(S_t^{(k)}) + w$$

where $F(\cdot)$is the solver of the discrete dynamics dislocation model, and w represents model error or stochastic model error. When the data of observation is obtained, the update step uses the Kalman gain to correct the states predicted.

$$K = PH^T(HPH^T + R)^{-1}$$

where P is the ensemble covariance matrix, H is the observation operator that projects out the observed dislocation node coordinates of the augmented state vector, and the result is projected into the observation space, and R is the covariance of observation noise. The new states of the ensemble turn out to be as

$$S_{t,\,\text{new}}^{(k)} = S_{t,\,\text{pred}}^{(k)} + K\left(y_t - HS_{t,\,\text{pred}}^{(k)}\right)$$

where y_t denotes the observation at time t.The update step jointly varies the dislocation configuration and the mobility parameters to make the predictions of the simulation consistent with the observation data. The ensemble average of the mobility parameters approaches the reference values as the assimilation cycles go on.

$$\hat{\theta} = \frac{1}{N_e}\sum_{k=1}^{N_e} \theta^{(k)}$$

The entire data assimilation process that brings together forward DDD simulation and EnKF parameter revision is represented in Figure 3, which depicts the iterative prediction error correction process in the estimation of the mobility parameter.

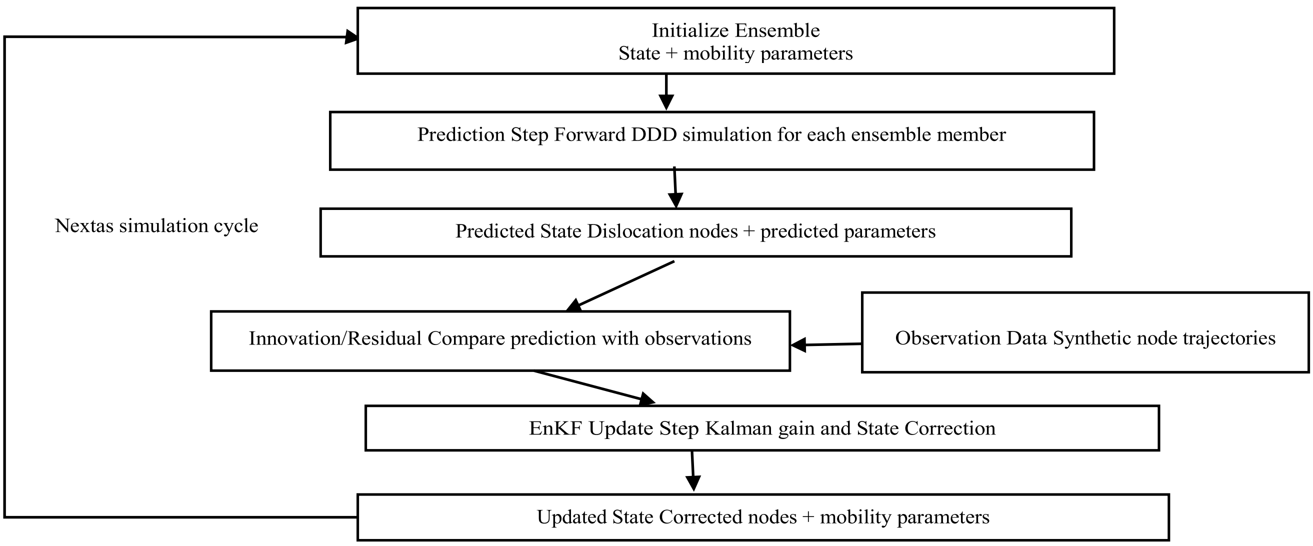

Fig. 3 Integrated inverse modeling framework combining forward DDD simulation with Ensemble Kalman Filter assimilation for mobility parameter estimation

Algorithm 1. EnKF-based Mobility Parameter Estimation

1. Initialize the ensemble of mobility parameters and dislocation node coordinates.
2. Run forward DDD simulation for each ensemble member.
3. Generate predicted node positions.
4. Compute the predicted observation vector.
5. Calculate ensemble covariance and Kalman gain.
6. Update ensemble states using observation data.
7. Update mobility parameters and dislocation node coordinates simultaneously.
8. Repeat the prediction–update cycle over successive assimilation steps until parameter convergence is achieved.

Otherwise, bold or vector-valued quantities represent state variables or observation vectors, and scalar variables represent mobility parameters, components of stress, or summary quantities obtained as a result of the assimilation procedure.

3. Results and Discussion

The numerical studies in this section test the performance of the proposed Ensemble Kalman filter-based inverse modelling system to determine various dislocation mobility parameters and approximate changing dislocation structure. Synthetic observation data generated by forward discrete dislocation dynamics simulations are used in the evaluation of the performance of the framework. Three dimensions are examined: convergence of the estimated mobility parameters, reconstruction of estimated dislocation configurations and stability of the framework to ensemble size, observation noise and initial parameter uncertainty.

3.1. Mobility Parameter Convergence

The overall aim of the suggested inverse modelling system is to determine the dislocation mobility parameters of screw, edge, and climb movements. Numerical experiments were used to assess the performance of the Ensemble Kalman filter (EnKF) using synthetic observation data that were produced by forward discrete dislocation dynamics simulations. The initial parameter estimates were known to be non-convergent to the reference values that had been used to obtain the synthetic observations to determine the convergence ability of the assimilation algorithm.

In the assimilation process, every ensemble member develops individually in the prediction step using a forward DDD model. The next step in the update process is to utilize the Ensemble Kalman filter, which takes into account the observation data used to correct the dislocation state variables as well as the mobility parameters, which are represented in the augmented state vector. With increasing iterations of the assimilation process, the ensemble average of the estimated values approaches the reference mobility values. At the same time, the ensemble spread reduces, which means that the uncertainty in the parameters is reduced because of the incorporation of observational data.

Figure 4 shows how the mean values of the screw, edge, and climb mobility parameters change during the assimilation process. The plots indicate a smooth optimization of the parameter estimates to the reference values applied in the synthetic simulations. This convergence behaviour shows that the EnKF-based inverse modelling framework can be used to simultaneously estimate several mobility parameters using consecutive observations of the positions of dislocation nodes.

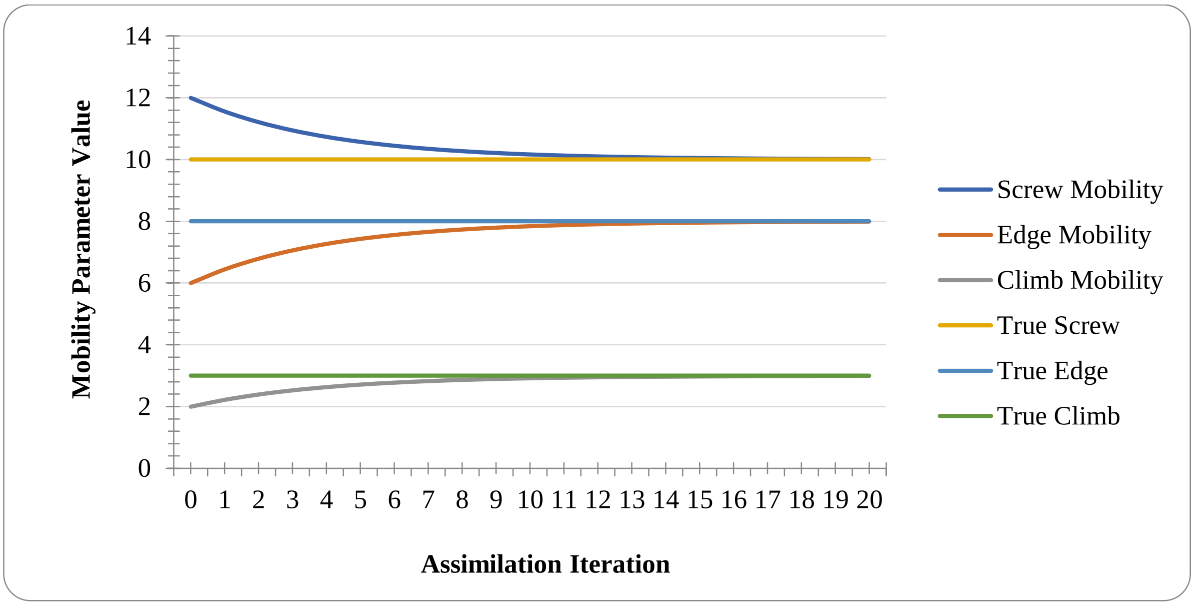

Fig. 4 Convergence of screw, edge, and climb mobility parameters during Ensemble Kalman Filter assimilation iterations

The last reference and estimated mobility parameters that have been obtained in the synthetic benchmark case are summarized in Table 3. The findings show that the approximate screw, edge and climb mobility parameters are similar to the reference values that were used to produce the synthetic observations.

Table 3. Mobility parameter estimation results

Parameter	True value	Estimated value	Relative error
Screw mobility	10.0	9.98	0.2%
Edge mobility	8.0	8.05	0.6%
Climb mobility	3.0	3.02	0.7%

Table 4. Estimated Parameter Uncertainty from Ensemble Statistics

Parameter	Estimated Mean	Standard Deviation	95% Confidence Interval
Screw mobility	9.98	0.08	9.82–10.14
Edge mobility	8.05	0.10	7.85–8.25
Climb mobility	3.02	0.05	2.92–3.12

Table 4 displays the ensemble statistics, with the standard deviations and 95% confidence intervals of all three mobility parameters being relatively small, and the parameter recovery and uncertainty in the estimation of the synthetic benchmark problem, which is the focus of the current research, are stable.

The small error in estimation, as shown in Table 3, is an indication that the proposed EnKF-based framework can be used to re-create a target mobility parameter set of the synthetic test case considered in this study. These results suggest that the assimilation method has the potential to estimate different dislocation mobility parameters simultaneously and utilize observation data to run the simulation process.

The decrease in ensemble diffusion shows that the mobility parameters can be determined using the existing node-trajectory measurements in the current synthetic benchmark conditions. The decrease in ensemble dispersion through the assimilation process is an indication that the mobility parameters can be determined based on the observed node-trajectory that is available.

Screw and edge mobility parameters have a little faster convergence to climb mobility than that of screw mobility, which implies that they have better observability in the loading conditions considered. This evidence suggests that the EnKF model would be dependable in estimating the three mobility parameters in the synthetic benchmark problem.

The proposed EnKF-DDD framework allows to automatically update of both the state variables and the mobility parameters, as well as to provide uncertainty estimates, in comparison with the traditional methods of DDD calibration, which often tend to rely on subsequent manual parameter optimization or trial-and-error optimization of mobility coefficients. The relative errors of less than 1% achieved in the synthetic benchmark case illustrate the potential of ensemble-based data assimilation to estimate multi-parameter mobilities with accuracy and less calibration effort and with greater robustness.

3.2. Reconstruction Accuracy of Dislocation Structures

Besides the estimation of parameters, the assimilation framework enhances the predictive accuracy of dislocation configurations by enhancing the observation data into the simulation procedure. Lack of assimilation means forward simulations with wrong mobility parameters cannot be the true dislocation structure.

This difference is corrected at the EnKF update step, in which the predicted node positions of dislocations are corrected with the help of observation data.

To assess the reconstruction accuracy of the structure of a dislocation, the Root Mean Square Error (RMSE) between predicted and observed node coordinates is used.

$$RMSE = \sqrt{\frac{1}{N}\sum_{i=1}^{N}\left(x_i^{pred} - x_i^{obs}\right)^2}$$

where N is the number of observed dislocation nodes, x_i^{pred} and x_i^{obs} are the predicted and observed positions of node i, respectively, at the same assimilation step.

A comparison of three dislocation configurations of the three refers to a synthetic observation structure, which created the observation data, the forward simulation result of the observation data without data assimilation, and the simulation result of the EnKF assimilation framework is shown in Figure 5. The forward simulation with no assimilation slowly loses its track with the observation structure as the incorrect mobility parameters have been utilised, and the simulation with the use of EnKF assimilation is very close to the observed dislocation structure. This comparison reveals that the assimilation framework is able to adequately rectify the adaptive dislocation geometry by assimilating the information of observation into the simulation.

Figure 6 shows the time-dependent behaviour of the reconstruction error that occurs as part of the assimilation process. RMSE values are reduced with successive steps of assimilation in which the state variables as well as the mobility parameters are updated. Such a decreasing of the RMSE means that there is better agreement of the predicted dislocation node coordinates with the observation data with the onset of the assimilation process.

The combination of the findings presented in Figures 5 and 6 proves that the framework suggested is better at estimating the mobility parameters and re-creating the accuracy of the reconstruction of the evolving dislocation structures using sequential data assimilation.

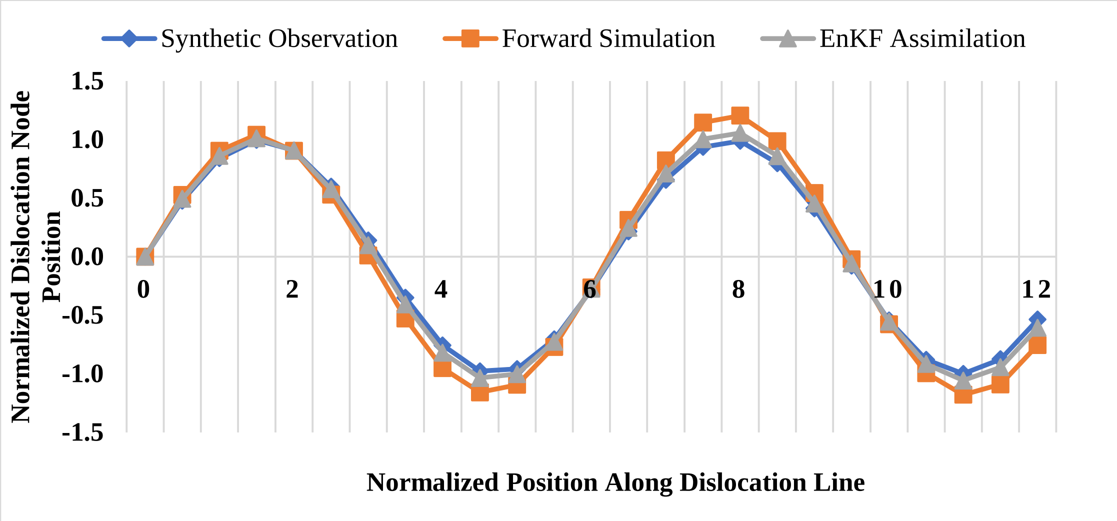

Fig. 5 Comparison of dislocation configurations for synthetic observation data, simulation without assimilation, and simulation with EnKF assimilation

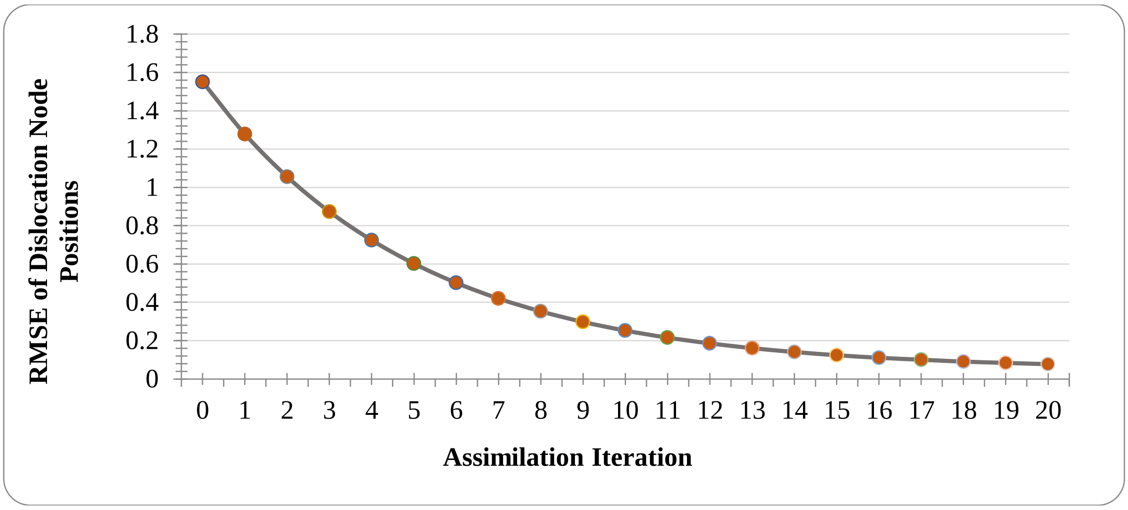

Fig. 6 Evolution of RMSE between predicted and observed dislocation node coordinates during assimilation iterations

3.3. Sensitivity and Robustness Analysis

Sensitivity analysis was done to test the strength of the proposed inverse modelling framework to major parameters like ensemble size, noise on observation, and initial uncertainty in the parameters. To begin with, they tested the dependence of ensemble size on the accuracy of parameter estimation using an ensemble size of 10, 20, 30, and 50 members. The results in Figure 7 suggest that the more ensemble members there are, the more the estimation process becomes stable, as it gives a superior approximation of the ensemble covariance that will be used in the Kalman update step. In the range of tests, the performance is less steep in the high ensemble size, suggesting a tradeoff between the stability of estimation and the cost. Second, observation noise was measured by adding to the sampled node coordinates a Gaussian noise (with increasing magnitude).

As anticipated, greater observation noise diminishes the direct concurrence between predicted and observed conditions at every assimilation step and may decelerate the stabilisation of the parameter approximations. However, the findings show that the assimilation model is still working with moderate levels of uncertainty of observation in the artificial environments that are taken into account in this research. Lastly, the strength of the ensemble with regards to uncertainty in the starting parameters was tested by initializing the ensemble using parameter guesses unrelated to the reference values with which the synthetic observations were produced. The findings indicate that larger initial deviations tend to need a longer assimilation path, at the end of which an ensemble mean comes close to the reference solution. Such a behaviour is in line with the sequential correction scheme of the EnKF and justifies the use of the approach to inverse problems, where it is only known that the initial estimates of the parameters are approximate. The general outcome of ensemble size and observation noise, concerning the error in parameter estimation, is provided in Figure 7. The findings show that the developed inverse modelling framework has a consistent performance in a broad set of simulation conditions. These findings suggest that ensemble sizes beyond 20 offer stable parameter estimation with only slight improvements as the size increases with respect to computational cost.

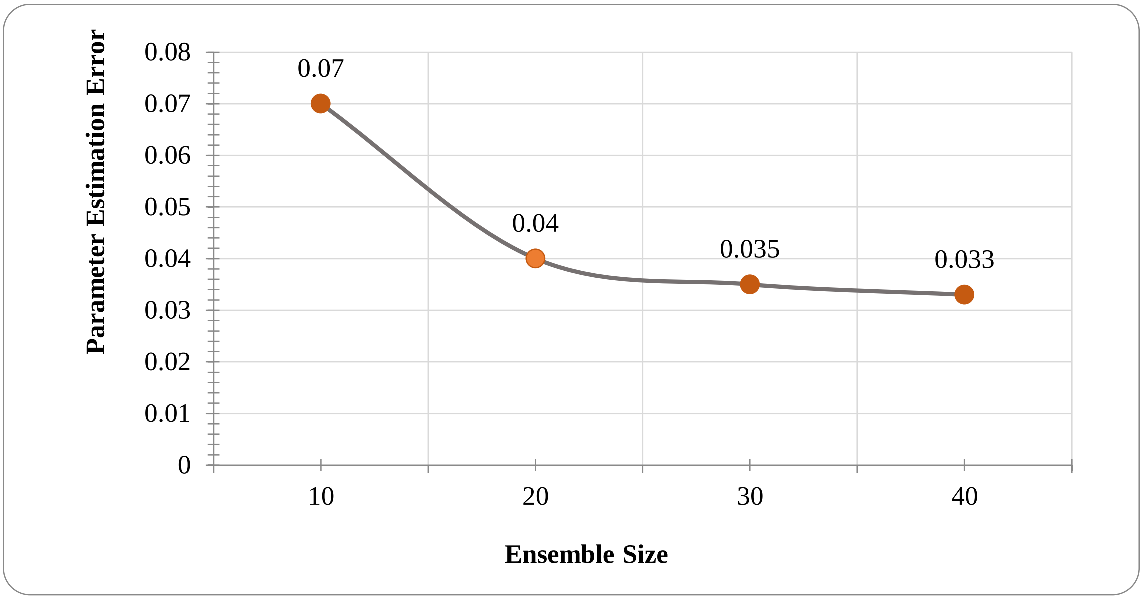

Fig. 7 Sensitivity of mobility parameter estimation accuracy with respect to ensemble size and observation noise.

It is important to note that the current validation is done on synthetic observations that have been created using the same DDD model used in the step of prediction. Although this controlled environment allows checking of the convergence of parameters, as well as the accuracy of estimations, this might not be the best representation of uncertainties in an experimental measurement. To somewhat overcome this shortcoming, the framework was tested in different ensemble sizes, noise in measurements and initial parameter uncertainties. Future research ought to take into account independent DDD configurations, different mobility laws, and experiments to further examine the generalizability of the proposed approach. The accuracy of parameter estimation with increased ensemble size is summarized in Table 5.

Table 5. Effect of ensemble size on parameter estimation accuracy

Ensemble Size	Screw Error (%)	Edge Error (%)	Climb Error (%)	Observation
10	1.8	2.1	2.5	Larger fluctuation
20	0.9	1.2	1.4	Improved stability
30	0.2	0.6	0.7	Stable estimation
50	0.2	0.5	0.6	Minor improvement

As Table 5 indicates, the accuracy of parameter estimates decreases, and the variability of the mobility parameters increases with the increasing ensemble size. Improvement is, however, marginal after an ensemble size of 30, meaning that larger ensembles might not only add much computational cost but also may not add much to the estimation performance.

Table 6. Computational setup used for EnKF–DDD simulations

Item	Description
Implementation platform	MATLAB/Python DDD–EnKF implementation
Processor	Intel Core i7 or equivalent workstation CPU
Memory	16–32 GB RAM
Ensemble sizes tested	10, 20, 30, 50
Default ensemble size	30
Parallel execution	Independent ensemble members can be advanced in parallel.
Main computational cost	Repeated DDD forward simulations for each ensemble member
Stopping criterion	Parameter convergence or final assimilation step

The computational cost of the proposed EnKF-DDD framework, summarized in Table 6, is mostly related to repeated forward DDD simulations of each ensemble member. Ensemble predictions are independent at the forecast stage, and so the framework can be easily implemented in parallel, which can save a lot of computational time with larger ensemble sizes.

4. Limitations and Future Work

Even though the suggested inverse modelling framework presents a consistent performance of the synthetic benchmark problems that are assumed in this work, quite a number of limitations must be considered. To begin with, the synthesis observation data used to validate the proposed framework in the paper is based on the same

Discrete Dislocation Dynamics (DDD) simulation model applied in the prediction step. Although this method allows one to overtly test the parameter estimation algorithm, experimental observations could present a host of new uncertainties in the form of measurement noise, imperfect observation of the structures of dislocations, and poor spatial resolution. Future efforts will involve incorporating experimental observations of the techniques, such as in situ transmission electron microscopy or electron tomography, in order to verify the framework under realistic experimental conditions. Second, the current model of mobility takes into account three independent parameters, which involve screw, edge, and climb dislocation mobility. Even though this simplified model describes the main anisotropic behaviour of dislocation motion, the real crystalline materials can exhibit more complicated mobility laws dependent on temperature, impurity concentration, local stress state, and crystallographic orientation. Future studies can also apply the inverse modelling framework to include temperature-dependent mobility laws and other physical processes so that one can more realistically model the microstructural evolution. Third, the existing model presupposes that the size of the discretized dislocation nodes is consistent between the state of the simulation and the observations. In realistic microstructure modelling, dislocation networks can be developed by dislocation multiplication mechanisms, dislocation annihilation mechanisms, or junction formation mechanisms, which can change the topology of the dislocation structure. Further studies in the field will involve more sophisticated node matching and node interpolation methods to account for the changing dislocation topology as the assimilation process unfolds. Lastly, the cost of computation of the proposed framework also grows with the number of ensemble members needed by the Ensemble Kalman filter. Even though ensemble simulations can be computed in parallel, the simulation of large-scale dislocation dynamics may demand significant computer resources. Future research will be done on reduced-order modelling, surrogate models, and adaptive ensemble strategies with the aim of enhancing the efficiency of the computations without losing the parameter estimation accuracy. Regardless of those restrictions, the findings that have been given in this paper exhibit that the combination of physics-based dislocation dynamics modelling with data assimilation methods offers a promising way of parameter estimation in microstructure modelling. Additional advances in integration experimentally and computer efficiency will allow the framework to be extended to the study of more complicated materials systems and on large scales.

5. Conclusion

This paper introduced an inverse modelling model to estimate dislocation mobility parameters in the simulation of the Ensemble Kalman Filter in discrete dislocation dynamics. The offered solution is a physics-based DDD forward model with an augmented-state sequential data assimilation solution where both mobility parameters and coordinates of dislocation nodes are updated in the course of the assimilation process. The framework was tested in control conditions using synthetic observation data.

The given numerical findings indicate that the given methodology is capable of not only restoring the reference screw, edge, and climb mobility parameters to the synthetic benchmark scenario that was taken into consideration in the current research but also enhancing the accuracy of reconstruction of the evolving dislocation configurations. The findings also show that the framework can be used when there is noise in observations and some initial parameter estimates are uncertain in the synthetic problems under test. The current research paper presents a demonstration of a workflow for identifying multiple parameters in microstructure-scale models. The next steps in the work should be the extension of the scheme to more multi-linear dislocation topologies, enhance the numerical report of uncertainty and cost of the calculations, and use the experimental reported data on observation to make the framework more comprehensive.

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