

Atomistic Modeling of Mg-Ion Implantation into GaN using an Efficient Machine-Learned Interatomic Potential

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Abstract—We present Mg-ion implantation and annealing simulations in GaN using a machine-learned interatomic potential based on the message passing atomic cluster expansion framework (MACE). Compared with empirical potentials, the MACE-based workflow yields more realistic defect recovery and defect distributions more consistent with experimental trends, providing a useful tool for analyzing defect evolution in Mg-implanted GaN.

Keywords—GaN, Mg doping, point defect, ion implantation, molecular dynamics simulation

I. INTRODUCTION

Ion implantation is a key technique for doping semiconductors due to its cost-effectiveness and reliability. Mg-ion implantation into wurtzite GaN is particularly important for power-device applications because it is currently the most practical method for selective p-type doping. However, achieving p-type doping by ion implantation remains challenging. Although a fraction of the implanted Mg atoms occupy Ga substitutional sites, vacancy-type defects generated during implantation can persist even after thermal annealing, limiting the achievable hole concentration [1,2]. At higher Mg doses, Mg precipitation can also occur [3]. The defect distributions produced by ion implantation depend on both the implantation conditions and the subsequent annealing conditions [2,4]. Despite extensive studies, the microscopic mechanism of Mg activation remains poorly understood because the evolution and interaction of implantation-induced defects during annealing have not been fully clarified.

Molecular dynamics (MD) simulation is an effective method for analyzing defect behavior at the atomic scale. To date, MD simulations of ion implantation into semiconductor crystals and the subsequent thermal annealing processes have mainly relied on empirical potentials, because the large number of atoms involved makes them impractical for calculations based on density functional theory (DFT) [5]. However, empirical potentials can yield markedly different predictions for the stability and diffusivity of crystalline defects, which may lead to inaccurate predictions of defect distributions. Although machine-learned interatomic potentials (ML IAPs) have enabled large-scale simulations with accuracy comparable to that of density functional theory (DFT) [6], a trade-off between accuracy and scalability

remains. Consequently, simulating ion implantation and subsequent annealing is still very challenging, as they require systems containing more than 100,000 atoms and robustness against thermally fluctuating, densely packed configurations.

In this study, we develop an efficient ML IAP for modeling Mg-ion implantation in GaN. We perform the MD simulations in a sequential workflow using the trained ML IAP together with an empirical ZBL potential to represent the strongly repulsive interactions at extremely short interatomic distances.

II. METHOD

The message-passing atomic cluster expansion (MACE) [7,8] was employed as the interatomic potential. By translating ACE's rigorous description of many-body correlations into the dynamic framework of message passing in deep learning, MACE enables the integration of high-order information while keeping computational costs low, resolving the trade-off between accuracy and scalability.

The MACE IAP was trained on cohesive energies and atomic forces computed with Quantum ESPRESSO [9,10] for 5,220 crystalline, amorphous, surface, and defective Ga-N-Mg configurations, including structures generated by MD and defect-diffusion calculations in LAMMPS [11]. Ultrasoft pseudopotentials and generalized gradient approximation for the exchange-correlation functional were used, where Gallium 3d electrons were explicitly included in the valence shell. The cutoff energy was set to 680 eV and the k -space mesh was set below $0.08 \text{ \AA}^{-1}$. All energy calculations were conducted under a neutral charge state.

The dataset was divided into training and test data in an 8:2 ratio. The cutoff length for the MACE model was set to 4.0 Å. To improve robustness for densely packed configurations encountered during implantation, we used the soft-type short-range interaction implemented in MACE.

III. RESULTS AND DISCUSSION

A. Training of the MACE interatomic potential

Figs. 1(a,b) compare the cohesive energies and atomic forces predicted by our trained MACE model with the reference DFT values. Almost all predicted energies fall within 0.3 eV/atom of the corresponding DFT values. The two data points underestimated by more than 0.3 eV/atom correspond to N-N dimer

configurations with two atoms in close proximity, and are therefore expected to have a negligible influence on the simulation results for defect behavior in GaN. The root-mean-square errors (RMSEs) on the test set for energy and force are 14.3 meV/atom and 220 meV/Å, respectively, and are comparable to those of the training set, indicating high accuracy and no serious overfitting.

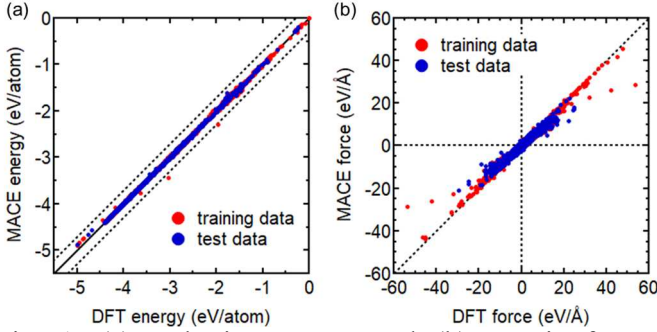


Fig. 1. (a) Cohesive energy and (b) atomic force comparison between DFT and our MACE model.

B. Formation energy of point defects

Formation energies of point defects in GaN were evaluated to validate the obtained MACE model. The formation energy $E(X)$ of a defect X in a neutral charge state was calculated as:

$$E(X) = E_{\text{tot}}(X) - \left[E_{\text{tot}}(\text{bulk}) + \sum_i n_i \mu_i \right] \quad (2)$$

where $E_{\text{tot}}(X)$ and $E_{\text{tot}}(\text{bulk})$ are the total energies of a point defect X and a perfect crystal GaN, respectively. n_i is the number of atomic species i added ($n_i > 0$) or removed ($n_i < 0$) from the pristine compound. μ_i is the chemical potential of the atomic species i .

The formation energy of each defect represents its relative stability compared with the perfect crystal. The defect distribution during post-implantation recovery is also expected to reflect the relative stability of each defect. In this study, we used $4 \times 5 \times 3$ supercells of a primitive GaN cell, with lattice constants a , b , and c obtained by geometry optimization in DFT as $a = b = 3.222$ Å and $c = 5.824$ Å, respectively. The k -space mesh in the DFT calculation was set to $2 \times 1 \times 1$. The chemical potential was set under Ga-rich conditions assuming equilibrium between Ga and GaN, and

between N and Mg_3N_2 . The energy was calculated after geometry optimization with fixed lattice constants. The atomic positions were relaxed until the maximum force on each atom was below 0.002 eV/Å.

Fig. 2 compares the formation energies of point defects in GaN, as calculated by DFT, trained and foundation MACE models, and an empirical potential. The empirical potential incorporates Tersoff/ZBL for Ga-N [12], ZBL for Ga-Mg and N-Mg [13], and EAM for Mg-Mg [14] interactions. The foundation model (MACE-MPA-0) has been developed as a pre-trained universal model [8] that serves as a general baseline for further training but is computationally more expensive than our trained model due to its longer cutoff length of 6.5 Å. The empirical potential is widely used to fully capture cascade collisions during Mg implantation. The formation energies obtained by DFT were in reasonable agreement with the reported results [15,16].

Our trained MACE model reproduced the DFT-calculated formation energies within a maximum deviation of 1.2 eV and an RMSE of 0.56 eV. In contrast, the MACE foundation model had a larger deviation of more than 2.7 eV with a larger RMSE of 1.6 eV. This represents a substantial improvement over the foundation model, which is attributed to our training focused specifically on defect configurations in GaN.

Although the empirical potential showed reasonable accuracy for interstitial and vacancy defects within 2.0 eV, it poorly reproduced antisite defects, with deviations exceeding 13.1 eV. In addition, because the Mg-Ga and Mg-N interactions are represented only by two-body interactions defined by the two-body ZBL potential and lack the angular three-body terms, the accuracy for Mg-related defects was also lower than that of MACE. These results suggest that the empirical potential may be limited in its ability to describe defect energetics in GaN.

C. Defect diffusion barrier energies

We further validated our MACE model by comparing diffusion barrier energies. Diffusion barriers of defects introduced by ion implantation influence the evolution of defect configurations during the fabrication process. We used the $5 \times 5 \times 3$ supercell of GaN and

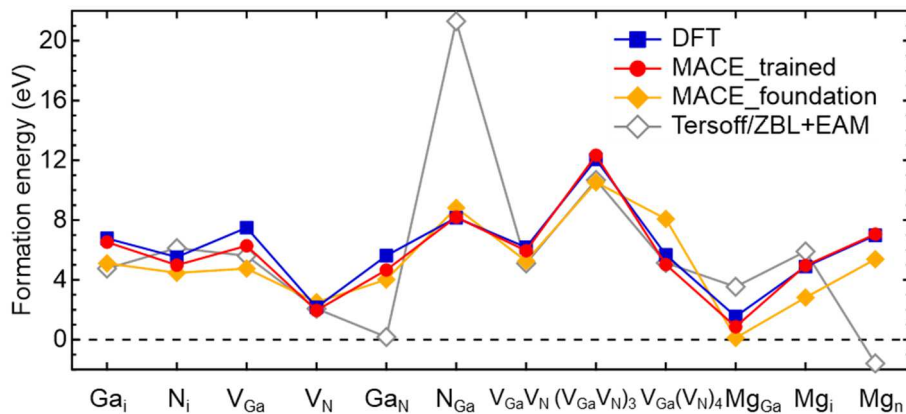


Fig. 2. Formation energies of defects in GaN calculated by DFT, trained and foundation MACE models and empirical potential (Tersoff/ZBL + EAM).

Nudged elastic band (NEB) method for the DFT calculations with the k -space mesh of $1 \times 1 \times 1$.

Dynamical evaluation more appropriately reflects defect dynamics during thermal annealing than the static NEB method. Therefore, the barriers for the trained and foundation MACE models were derived from Arrhenius plots of the mean-square displacement (MSD) obtained from MD simulations. However, for the empirical potential, the NEB results are shown because the N interstitial defect did not form the split-interstitial configuration during finite-temperature MD simulations.

Fig. 3 shows the defect diffusion barrier energies in GaN. MD simulations for the MSD analysis were performed over a temperature range from 1650 K to 2750 K for interstitial defects and up to 3250 K for vacancy defects. For interstitial defects, higher-temperature data were excluded because the diffusion trajectories changed to different mechanisms, which also changed the Arrhenius slope. The timestep was set to 1.0 fs, and the simulation time was 1 ns. To reduce fluctuations in the time evolution of the MSD, each MD trajectory was divided into 50 ps segments, and the slope of the MSD with respect to time was obtained from the averaged trajectories and used for the Arrhenius plots [17]. The DFT-derived values are in good agreement with previous reports [18,19]. The foundation model exhibited a maximum deviation of 0.8 eV from DFT and an RMSE of 0.48 eV. In contrast, our model achieved a maximum deviation of 0.3 eV and an RMSE of 0.13 eV, indicating that it more accurately reproduces the relevant energy landscape under thermal fluctuations. The empirical potential showed an even larger deviation of 9.1 eV and an RMSE of 4.2 eV, indicating that it does not adequately capture the underlying energy landscape. For the empirical potential, these NEB barriers should be interpreted qualitatively because smooth single-peak migration profiles were not obtained for Ga_i and Mg_i , and N_i did not retain the split-interstitial configuration during finite-temperature MD. Therefore, the empirical barriers indicate a distorted energy landscape rather than reliable diffusion kinetics.

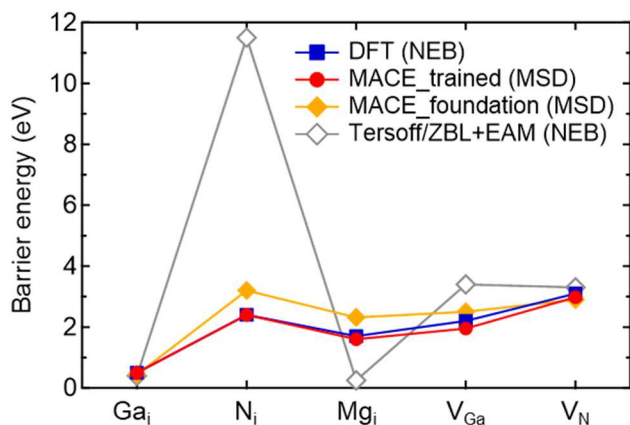


Fig. 3. Defect diffusion barrier energies obtained from DFT, trained and foundation MACE models and the empirical potential.

D. Mg implantation and annealing simulations

We performed Mg implantation simulations in a $78 \times 81 \times 220 \text{ \AA}^3$ GaN slab model containing 100,800 atoms [Fig. 4(a)]. The bottom layer of GaN was fixed during the simulation. Sixty Mg atoms accelerated to 2.5 keV were injected at a 7° tilt, corresponding to a dose of $9 \times 10^{13} \text{ cm}^{-2}$, which is typical for experiments. Following the multi-stage approach shown in Fig. 4(b), we first used the empirical potential composed of Tersoff/ZBL and EAM potentials to capture cascade collisions during Mg bombardment, while including electronic stopping and adaptive timesteps. The MACE foundation model was not used in this stage because its longer cutoff length makes the computational cost impractical for the present large system. The initial temperature was set to 293 K. The 25 $\text{\AA}$ region from the bottom surface was controlled as a thermostat region using a Berendsen heat bath, whereas the upper region was treated with the NVE ensemble. After each Mg injection, the simulation was continued for 40,000 steps until the collision cascade ended and the system relaxed, which corresponded to 7–11 ps depending on the channeling. Mg atoms that channeled into the thermostat region were removed, accounting for less than 20% of the injected atoms. After the ballistic cascade stage, the atomic configuration was transferred to MACE for a short relaxation with 4,000 adaptive timesteps followed by 4,000 fixed timesteps of 0.5 fs under the NVT ensemble. This process cooled the system below 400 K and relaxed structures that were physically unstable but had been artificially stabilized by the use of Tersoff/ZBL.

Figs. 4(c,d) show cross-sectional views after implantation using Tersoff/ZBL alone and the sequential Tersoff/ZBL plus MACE workflow, respectively. The short relaxation using MACE reduced the distorted region. Figs. 4(e,f) show the corresponding cross-sectional views after 2 ns annealing at 1873 K using the different potentials under the NPT ensemble. The system was heated to 1873 K with a timestep of 0.5 fs at a rate of 20 K/ps and was cooled back to 293 K at the same rate after annealing. The timestep was increased to 1 fs only during the holding stage at 1873 K. Although 1873 K is high enough to cause surface degradation experimentally in the absence of N_2 overpressure, it was selected to accelerate defect reactions within the short timescale accessible to MD. The slab structure was maintained throughout the 2 ns annealing simulation. Although annealing healed the distorted regions regardless of the potential type, the MACE IAP appears to enhance defect recovery. This behavior is consistent with the more accurate defect energetics and diffusion barriers predicted by MACE, leading to more realistic post-implant annealing behavior and enhanced Mg_{Ga} formation.

To quantify the defect distribution, we counted the representative point defects shown in Fig. 5. V_{N} was the most abundant defect regardless of the potential type,

which is consistent with its low formation energy. The MACE IAP promoted the recovery of all vacancy-type defects and the formation of Mg_{Ga} . The predominance of $V_{\text{Ga}}V_{\text{N}}$ over V_{Ga} is indicative of the initial stage of defect recovery [1,2], supporting the physical realism of the IAP and the overall simulation procedure.

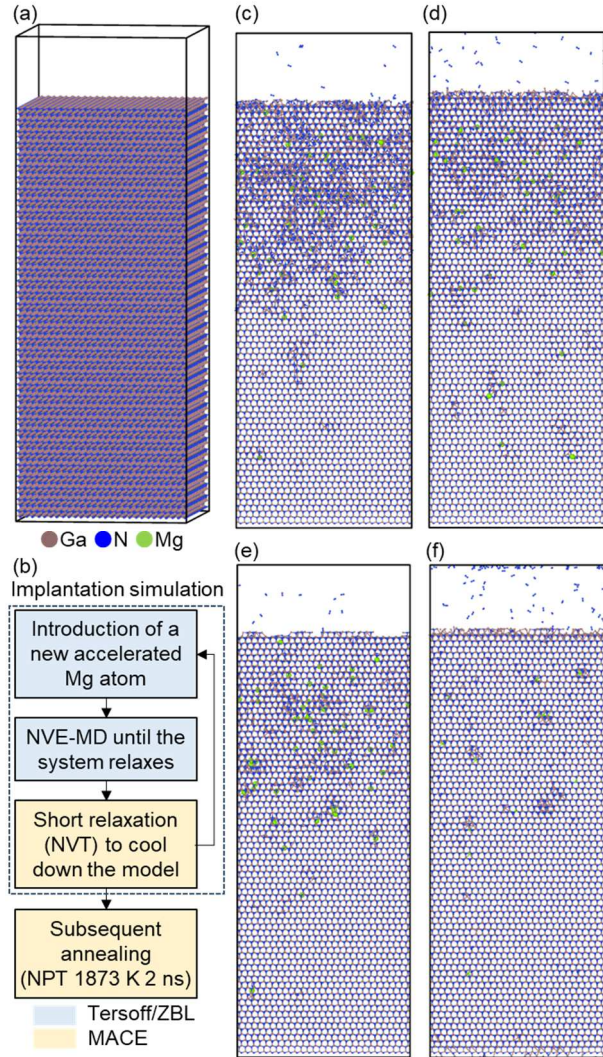


Fig. 4. Mg implantation and annealing workflow in GaN: (a) initial GaN(0001) slab model; (b) multi-stage simulation workflow; (c,d) cross-sectional structures after implantation using Tersoff/ZBL alone and sequential Tersoff/ZBL plus MACE, respectively; (e,f) the corresponding structures after 2 ns annealing.

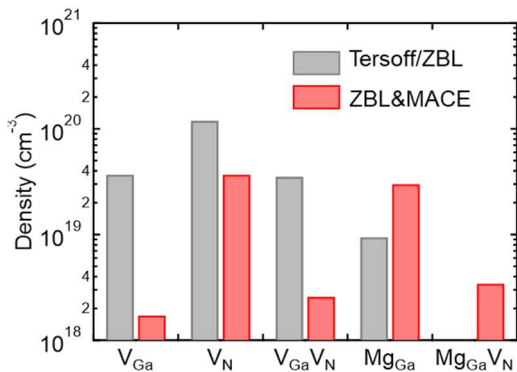


Fig. 5. Density of point defects after 2 ns annealing.

IV. CONCLUSION

In this work, we developed a MACE IAP for Ga-N-Mg systems with high accuracy and scalability. Mg implantation simulations in GaN using this potential yielded defect distributions that are more consistent with experimental trends, providing a valuable tool for understanding and optimizing Mg doping processes.

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