

Deep Neural Network Application to Real-Time Growth Prediction of Epitaxial GaN by Molecular Beam Epitaxy

Giovanni Drera,* Stefano Vichi, Matteo Canciani, Richard Nötzel, and Stefano Sanguinetti



Cite This: <https://doi.org/10.1021/acs.cgd.6c00850>



Read Online

ACCESS |

Metrics & More

Article Recommendations

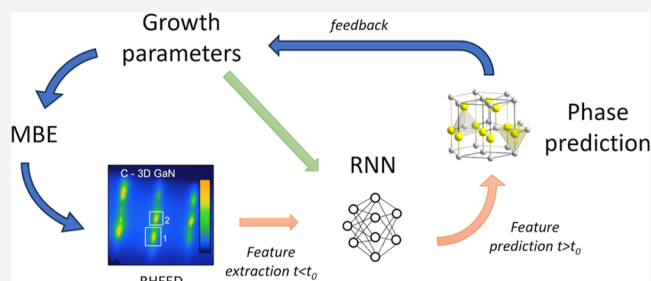
Supporting Information

ABSTRACT: In this work, we explore the application of machine learning (ML) methods, specifically recurrent neural networks (RNNs), for the analysis and prediction of GaN growth via molecular beam epitaxy (MBE). In particular, we show the possibility to control in real-time and predict the growth evolution based on the actual values of selected parameters. For this purpose, we tailored a specific GaN growth sequence, derived from droplet epitaxy and metal modulated growth; each deposition is characterized using the surface morphology information contained in the reflection high-energy electron diffraction (RHEED) images together with relevant MBE experimental parameters, such as nitrogen flux, power, and cell temperature. The classification and prediction nets work collecting data on an input window of about 10 s and provides a good prediction accuracy (> 0.90) over a similar time horizon, with a small sized, fast RNN. The simplicity of this net allows for real-time control of the MBE growth, while at the same time providing an early alarm system for unwanted secondary phases through the growth predictions.

KEYWORDS: reflection high energy electron diffraction, molecular beam epitaxy, machine learning, recurrent neural network

INTRODUCTION

Molecular Beam Epitaxy (MBE) represents a fundamental crystal growth technique, enabling the synthesis of semiconductor materials with atomic-level precision. Unlike Chemical Vapor Deposition (CVD), which relies on the thermodynamic equilibrium of precursor gases, MBE is a kinetically controlled process. This allows for the fabrication of nonequilibrium alloy compositions and complex heterostructures that are critical to modern optoelectronics and high-mobility electronic devices.^{1,2} However, just because MBE operates in a kinetic regime where adatom incorporation is a competitive process between ordered epitaxy and entropic roughening, static calibration is insufficient. The conditions to achieve high-quality epitaxial layers are precarious. If the adatom mobility is insufficient relative to the flux rate, a transition to a roughened growth mode (kinetic roughening) compromises the quality of the epilayer and in turn the abruptness of heterojunction interfaces. Because the system is far from thermodynamic equilibrium, it possesses no intrinsic restoring force to correct these morphological defects once they occur; consequently, active external control based on real-time kinetic data is required.³ A fundamental advantage is related to the high-vacuum environment of MBE, which permits the use of electron beam diagnostic tools, like reflection high energy electron diffraction (RHEED), during the growth process, a capability not possible in gas-phase reactors. RHEED has the ability to give real-time information on surface crystallography and its evolution during the growth. RHEED patterns provide valuable information regarding growth modes,



surface reconstructions, and growth rate, all of which are crucial information required to achieve high quality epitaxial layers.^{4–6} Despite its critical importance, the analysis of RHEED is generally carried out manually by operators based on the direct observation and interpretation of the diffraction pattern. This approach makes it difficult to extract quantitative information in real time and makes it almost impossible to identify subtle changes in the surface morphology which can lead to undesired results later on during the growth. While the human eye is not capable of promptly recognizing small changes in RHEED patterns before they lead to irreparable effects, applying machine learning (ML) algorithms has the potential to completely solve this issue and gather deeper information.

In particular, being able to apply ML algorithms to RHEED monitoring represents a revolutionary advancement in epitaxial growth control, offering the capabilities for automated pattern recognition, growth phase classification, and predictive modeling. In this work, we are pioneering the use of neural networks to identify in real time the growth phase and to predict surface morphology transitions, providing reliable and quantitative metrics for growth control.

Received: June 17, 2026

Revised: September 17, 2026

Accepted: September 21, 2026

ML methods have already been applied to analyze RHEED data. ML methods have been used in order to identify important features or underline specific areas-of-interest on RHEED images. Liang et al.⁷ developed a tool to identify relevant RHEED features such as streak and spots through the application of deep neural networks (DNNs). Furthermore, ML methods can be used for the direct classification of ingrowth surface phases through supervised⁸ and unsupervised⁹ classification methods. In this context, pre-trained models, such as AlexNet¹⁰ or VGG16,⁹ have been applied in order to extract features for each single RHEED image, which can then be classified in real-time through various algorithms. Such results can be used in order to track or design better growth strategies; for instance, ML fast featurization and classification algorithms¹¹ have been applied in order to predict the stoichiometry of V-doped WSe₂ from RHEED data; genetic algorithms have been applied for the stoichiometry control of Al_xGa_{1-x}As MBE growth through ellipsometry;¹² finally, Shen et al.¹³ applied automated ML RHEED analysis for actual real-time control of InAs/GaAs quantum dot growth.

Few works have been devoted to the actual prediction of the crystal phase evolution during an MBE growth. In this work, we explore the predictive capabilities of DNN applied to RHEED camera streams, in order to allow not just for real-time growth control (i.e., real-time assessment of the surface state), but for actual growth phase forecast. This expert system, which also accounts for actual MBE growth parameters, also acts as an early warning system for the whole growth process, which can be used to halt the growth in order to reduce the risk of unwanted secondary phases.

For this study, we chose to analyze the growth of GaN, due to its relevance for applications in electronics and optoelectronic devices,^{14–20} which are all extremely sensitive to growth quality. Moreover, GaN epitaxy would benefit enormously from this implementation, as the parameters space to achieve optimal growth conditions is particularly narrow at typical MBE growth temperatures when high growth speed is targeted.^{21–23} Indeed, due to the low diffusion length of N atoms on the surface at typical MBE growth temperature, a metal Ga adlayer is generally required to act as a surfactant and improve the smoothness of the growth.^{24,25} Maintaining this equilibrium is particularly difficult for long growths, as even a slight excess of Ga will result in droplet formation and, on the other side, a N excess will lead to 3D growth. Even the change in surface temperature with epilayer thickness affects this delicate balance. To prevent these conditions, the growth of 2D GaN is typically achieved by interrupting the growth after a few tens of minutes to adjust the growth parameters and go back to the optimal conditions. Others chose a different approach called metal-modulated epitaxy, in which the growth is achieved by alternating Ga deposition and crystallization cycles in order to increase growth speed, migration length, and reduce temperature.²⁶ Clearly, both approaches are just workarounds to limit the negative impact of the inevitable drift in the growth conditions.

MLbased RHEED analysis has then the potential to revolutionize semiconductor manufacturing by enabling fully autonomous growth control systems that can respond in real time to subtle changes in growth parameters, predicting phase transitions before they become evident, and responding by keeping the optimal growth conditions. This innovative approach represents a critical step toward intelligent manufacturing systems that can consistently produce high-quality semiconductor materials with unprecedented precision and reliability.

METHODS

GaN growth

The GaN growth was performed in a Riber 32 MBE machine, equipped with a double filament Knudsen cell for gallium evaporation and a high-density radical source (HDRS) radio frequency plasma cell from Hakuto for the active nitrogen supply. On the back of the plasma source, a silicon photodiode was mounted to measure the plasma emissivity, which gives an indication of the amount of active species.²⁷ The MBE was equipped with a thermocouple mounted on the back of the sample to measure substrate temperature, an optical pyrometer, and a standard RHEED equipment. For the growth, a commercial *c*-plane GaN on the sapphire template grown by MOCVD was used. It was cut in a square of 18 mm side and it was back coated with a 100 nm titanium layer to improve heat absorption. Before growth, it was degassed in the load-lock chamber at 250 °C overnight at a base pressure below 10^{−8} Torr. The substrate was then moved to the main chamber and thermally cleaned by heating it up to 700 °C for 10 min at a base pressure of approximately 10^{−10} Torr. Next, the substrate temperature was increased up to 775 °C to remove the native oxide by depositing Ga for 10 s at a beam equivalent pressure of 2 × 10^{−7} Torr and waiting for it to desorb while monitoring RHEED.²⁸ After cleaning the substrate, the temperature was decreased to 700 °C, ensuring a negligible Ga desorption, and it was kept constant for all the next steps.

The data was collected for various GaN deposition cycles, which usually last about 100 s, for a total time of approximately 6000 s. Data collection was performed in 13 different data sets, each comprising different phase transitions with different growth conditions. In detail, the gallium temperature was changed between 922 °C and 960 °C, corresponding to beam equivalent pressures in between 1.1 × 10^{−7} Torr and 2.2 × 10^{−7} Torr, respectively. The nitrogen plasma power was changed between 300 W and 600 W, whereas the flux was changed between 1 sccm and 5.5 sccm. RHEED images, Ga cell temperature and shutter state, and N source data and substrate temperature have been tracked during each acquisition. RHEED images have been averaged in a 0.5 s window, which in our case provides a good compromise between accuracy and signal noise.

Data Collection

In GaN growth dynamics, each RHEED frame, averaged in a time window of 0.5 s, usually provides two main indications about the state of growth: (i) an overall dimming of the whole diffraction pattern, which is ascribed to the presence of metallic Ga on the surface,^{26,29} and (ii) the appearance of additional peaks, which are usually related to the shift of the growth towards a 3D mode⁴ (see markers 1 for 2D and 2 for 3D in Figure 1f). We obtained the intensity information (*I*_{RH}) on the RHEED frames by averaging the data outside the main peak positions, to avoid sensor saturation problems, and extracted the ratio (*R*_{RH}) of 2D and 3D peaks by means of curve fitting.

A plot of data from a single acquisition run is shown in Figure 1. In this particular data set, several growth cycles have been performed with different growth conditions, namely different plasma power and nitrogen flux (Figure 1a,b). Growth cycles are started by the opening of the Ga cell shutter (Figure 1c), which usually results in the dimming of the RHEED frames due to a III/V ratio larger than unity; after Ga shutter closing, the crystallization proceeds by consuming the excess Ga on the surface, detectable as a modulation of both intensity and peak ratios. During normal operations, nitrogen plasma is usually kept on continuously, although with variable power and flux. Together with the flux and the plasma state, we also tracked the plasma emission intensity through a Si photo diode (Figure 1a), which is able to capture subtle plasma oscillations, drift, which otherwise could not be identified by plasma power, and nitrogen flow parameters, which are fixed. RHEED extracted features are shown in Figure 1d. Here, labeling has been performed by experienced MBE operators, through a combination of careful RHEED sequences and MBE parameter evolutions analysis; we expect to have an average accuracy of about ±2 frame for phase border detection. Together with the usual transition 2D – liquid Ga – 2D, an additional indication to a 3D-like growth can be detected (C marker),

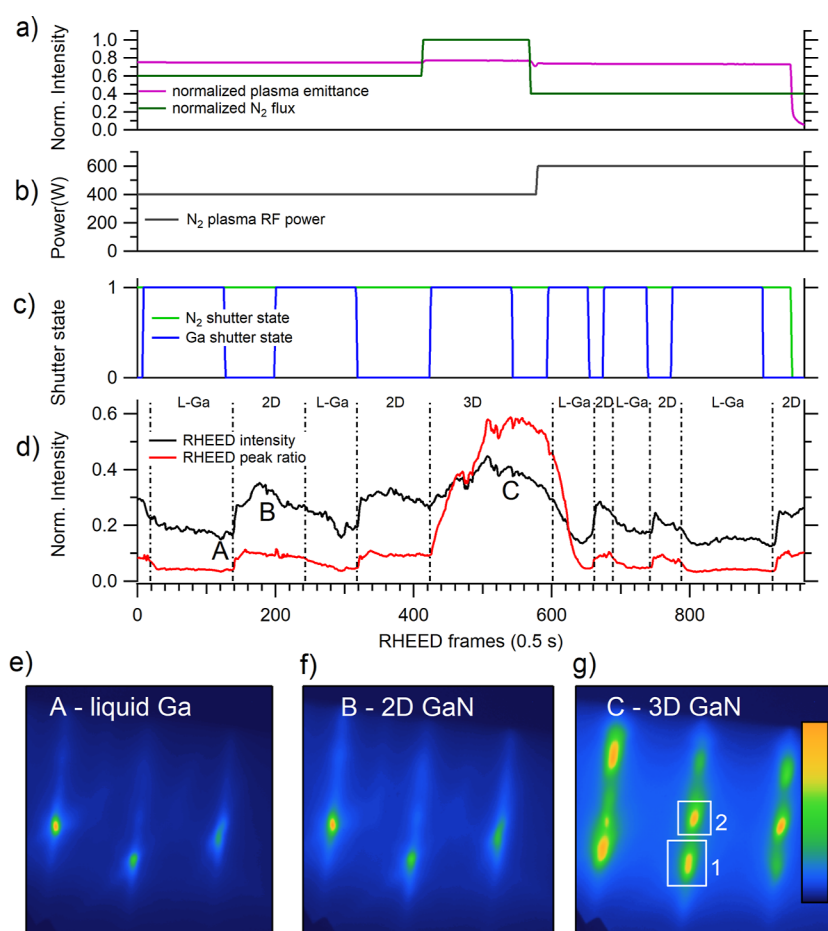


Figure 1. (a,b,c) Experimental parameters collected during a MBE GaN growth run; (d), normalized RHEED extracted features; and (e,f,g), RHEED frames collected at positions A,B and C in panel (d).

induced by an excess of N₂ flux. Such transition can be clearly seen in the RHEED frames (Figure 1e,f,g) and subsequently in the extracted R_{RH} (corresponding to A, B, and C markers in Figure 1d).

The onset of any phase is not just determined by the Ga shutter state change. For instance, the 2D or 3D crystallization can trail the closing of Ga shutter of several seconds, while the RHEED dimming effect can be delayed with respect to the Ga shutter closing. In general, several additional factors are expected to be relevant for the growth dynamics, such as the previous Ga deposition time (which determines the total amount of liquid Ga available for crystallization) and recrystallization time (which determines how much residual Ga is left on the surface); we thus expect the growth to be also dependent on the history of the surface deposition. It is often difficult to directly measure or predict the surface evolution by theory alone; for this reason, we provide a better estimate of growth dynamics through large data accumulation and machine learning.

In summary, the list of the additional experiment parameters considered for the forecasting is the following.

- N_s : nitrogen shutter state (encoded as a binary 0,1 state);
- N_f : nitrogen flux;
- P_{RF} : plasma power;
- P_e : plasma emissivity;
- G_{AT} : gallium effusion cell temperature;
- $G_{s(t)}$: Ga shutter state.

All these parameters have been encoded in a $[-1, 1]$ interval for subsequent neural network application. These parameters have been selected for two main reasons: i) their relevance for the actual growth evolution and ii) they are often actively tuned by the MBE operator in order to achieve optimal performances.

For the gallium cell shutter state, which is a critical parameter, instead of adopting a simple binary encoding as the nitrogen one, we calculated a cumulative parameter.

$$G_{s(t)} = \pm \tanh \frac{t}{\lambda} \quad (1)$$

which depends on the temporal frame delay t from the previous shutter state change. The positive and negative branches of eq 1 define the opening and closing of the shutter, respectively; positive $G_{s(t)}$ are related to Ga deposition, while negative values usually corresponds to Ga crystallization phases (2D and 3D). The decay parameter $\lambda = 25$ s has been chosen according to the typical deposition timescales in our system. This choice for the Ga encoding stems from the particular problem addressed by this work, which is a growth evolution forecast based on the measured previous growth states. This type of encoding contains not only the information about the instantaneous Ga shutter state (the function sign) but also about the time interval from the previous shutter change. In such a way, we can perform a future forecast with a significantly reduced measured data set, with an obvious reduction of computational cost and a better execution speed. Result comparison for identically sized networks and different Ga shutter parametrization (see Supporting Information, Figure 3d) clearly shows much better results with the introduction of eq 1.

In order to provide good metrics for the future state prediction, we also designed a simple classification model based on I_{RH} and R_{RH} and on $G_{s(t)}$ parameters. Full details are given in Supporting Information S1. The inclusion of $G_{s(t)}$ allows for a better discrimination between liquid Ga and 2D/3D phases, due to the inclusion of the shutter state.

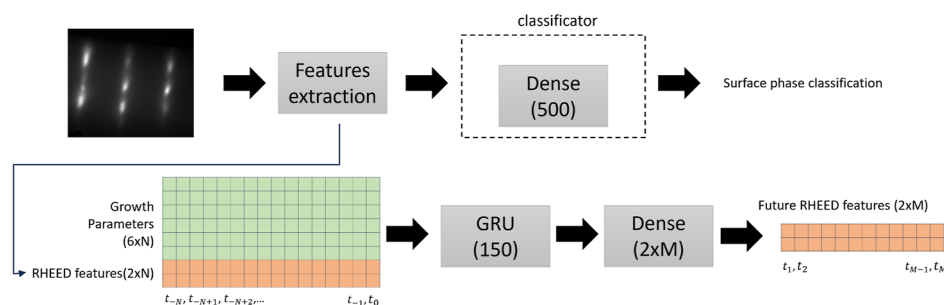


Figure 2. Classification and prediction net layouts. The RNN predicts M future RHEED features starting from N previous ones with additional MBE parameters. The classification net is not trained together with the prediction one.

Data Modeling

Since our data set is time ordered, we resorted to recurrent neural network design, and in particular to gated recurrent units (GRU)³⁰ as implemented in Tensorflow). The layout of the net is shown in Figure 2. The classification module has been applied to native data and to feature prediction, in order to assess the net predictive power (through classification metrics) together with the feature prediction quality (through standard L_2 norm).

For each iteration, we consider N previous frames (each corresponding to a 0.5 s interval) in order to predict M future RHEED features, with $M \leq N$; models are then identified by (N, M) labels. External parameters are supplied as additional net inputs but are not predicted by the RNN; in fact, this model should predict the evolution of a system under the assumption of constant MBE parameters. GRU has been selected because of the time-ordered nature of input and output data, in order to reduce the number of required hidden trainable units. Given the limited feature size and the application of GRU, a minimal net of about 150 units, corresponding to 80 k parameters, is enough for the prediction task. We stress that this result is only attainable due to the limited RHEED feature extraction size; we expect that the direct application of a full RHEED image stack would lead to rather large NNs and increased computational requirements. A comprehensive description of training process and accuracy results is shown in Supporting Information, S1.

RESULTS

An example of feature predictions is given in Figure 3 for net (18,15) for both the validation set and a training run. All $M = 15$ future features are depicted for each reference time, creating a sparse point cloud which is expected to follow to the ground truth values. Predictions at selected t are highlighted as bordered dots. Results are visually satisfactory for both the training data (Figure 3a) and the training set (Figure 3b). Please note that this static representation of dynamic predictions is quite difficult; we suggest the reader to visualize more graphs and live animations in the Supporting Information for selected nets. Accuracy is particularly good for R_{RH} (yellow traces), suggesting a better performance in predicting the 3D growth phase. However, as pointed out in Figure 3d (which is a detail of Figure 3b in the position marked by the corresponding arrow), predictions are wrong when a substantial state change (in this case, the Ga shutter opening) is happening in the future time span, and thus a phase transition cannot be predicted by the DNN. This is expected in our approach, and it is actually a good proof of a sound model training without overfitting to a specific data set. When the shutter state change is incorporated in the net input (such as for Figure 3c), a good agreement with experimental data is found.

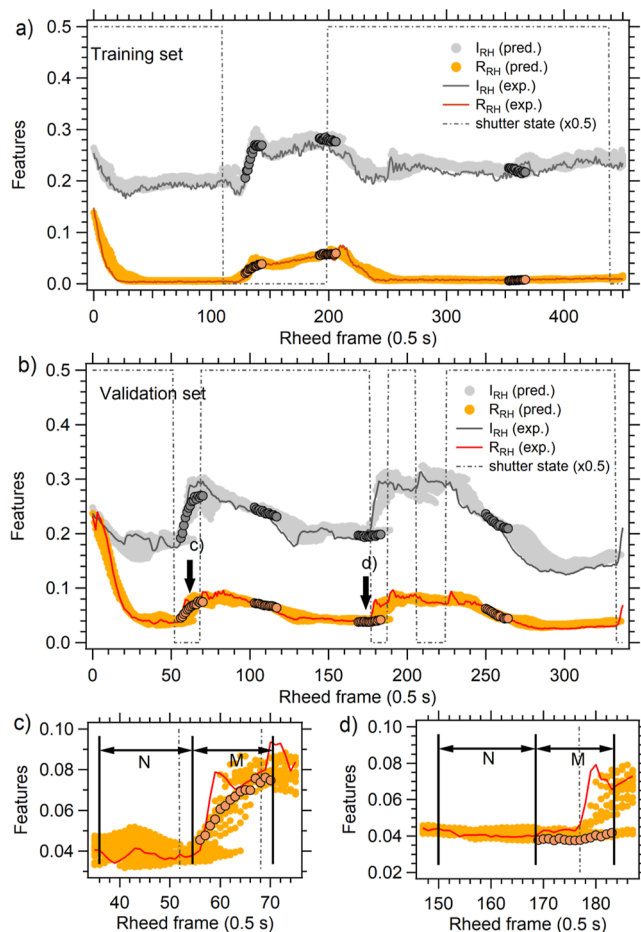


Figure 3. (a,b) Net (18,15) predictions (I_{RH} and R_{RH} , filled circles) together with experimental features at t_1 (solid lines); results are given for the validation set (a) and for a subset of training data (b). The Ga shutter state is shown as a dotted gray line for reference; selected single predictions are shown with bordered markers. (c,d) Details of data shown in panel (b) on areas located by corresponding black arrows.

In order to assess the actual capability of a model (N, M) to predict the growth phase, we applied the classification net to the farthest prediction (t_M). The result is then compared with the expected class at the same frame time, through standard classification metrics. A summary of final results is shown in Figure 4 (frame-resolved loss scores and additional f1 metrics are shown in Supporting Information, S3). As expected, the accuracy is decreasing at higher prediction depth; yet, accuracy at the larger depth considered,^{18,24} is still 0.90.

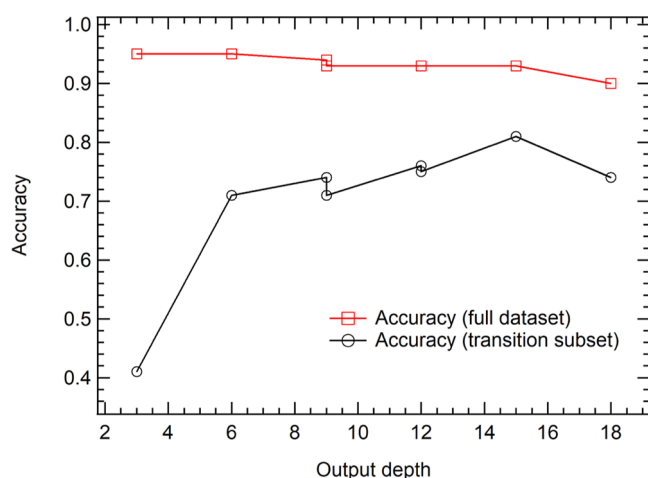


Figure 4. Accuracy scores for the full data set and the phase transition limited data subset as a function of the total output depth M . Full f_1 scores are given in the Supporting Information.

It should be noted that, for most data points, the system actually stays in the same phase in the M future frame interval. To better assess our model quality, we considered also a naive classification, where the predicted class is identical to the initial one, and a linear classification, where the features at t_M are obtained as a linear extrapolation in the interval $t = [t_N, t_0]$. As expected, all these models gave good average results, with an accuracy for model^{12,18} of about 0.93 and 0.90 for the naive classifier and the 0.91 for the linear interpolation.

However, for practical application, the prediction net should perform well when a phase transition is actually happening. We then performed an analysis on the data subset with an ongoing phase transitions, i.e. where the class at T_0 and T_M are different, reducing the actual data support from 9500 to about 1100 samples. In this subset, the naive classification obviously fails at every data point. RNN models accuracy results are shown in Figure 4 (circles), labeled transition subset. As expected, the overall accuracy is reduced as compared to the full data set, especially for short depth prediction. We found a 0.81 maximum accuracy for the^{15,18} net, which is an acceptable result for practical applications. As a comparison, the linear interpolation classification applied on $[t_{-18}, t_0]$ display an accuracy of 0.24. Other classification models, such as a properly-trained Random Forest classifier (more details in the Supporting Information), can achieve a similar (0.70) accuracy on the transition subset. Our GRU model provides similar or better performances, while also providing full predictions (regression and classification) for all features in the prediction window. Please note that the overall results are still affected by the model limitations, and in particular when shutter state changes are included in the prediction time span (as already discussed for data in Figure 3d), thus slightly decreasing the overall accuracy figures.

Summing up all the results, we then consider as the most effective nets for phase detection the (18,15) and (18,12) cases. These models can then provide a reasonable 6–8 s early alarm system in case of unexpected phase transitions and could thus be used as expert systems for active control of the growth process. The predictions can be obtained in real-time, due to the lightness of the neural networks involved; actually the same model can be performed several times within a range of external parameters, in order to calculate the possible net outcomes with various MBE configurations.

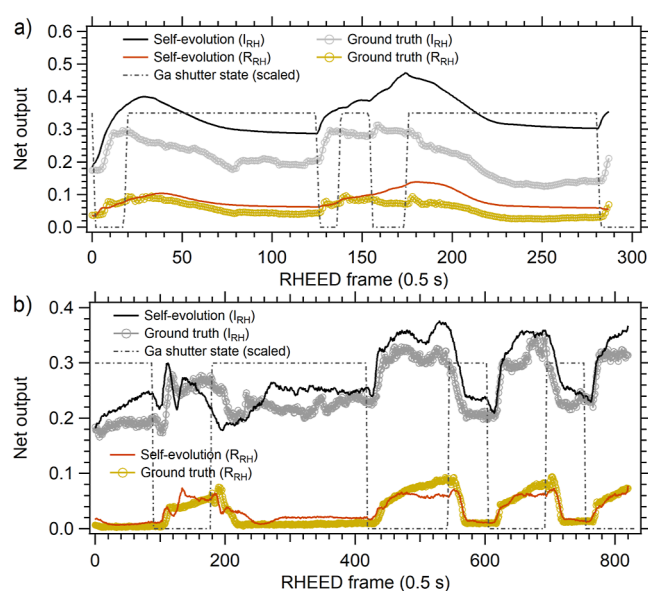


Figure 5. Self-evolution of initial parameters for the validation data set (black and red lines) compared to the ground truth values (orange and gray lines): (a) the validation set and (b) a training set. The scaled Ga shutter state is given as a reference.

In this context, we tested the net capability to actually simulate an entire data set just from a starting RHEED feature set. Examples are shown in Figure 5 for nets (18,15) and (18,12), other self-evolution examples are provided for selected models in the Supporting Information. In these simulations, the MBE parameters have been adopted from the validation data set, while only the first 18 I_{RH} and R_{RH} data points have been used as the net seeds; the intensity and peak ratio evolution is simulated for the full set by using the net output as the input for each subsequent iteration. Of course, we expect a cumulative error to be propagated during the simulation. While the absolute values differ from the ground truth, the modulation of both I_{RH} and R_{RH} are extremely well reproduced; as expected, the self-evolution is slightly better for a training set (Figure 5b) with respect to the validation one (Figure 5a). This good agreement suggests that an improved model based on this work, with a larger data set and a wider range of parameters and features, could be effectively used as a state machine for a MBE growth process.

CONCLUSIONS

In conclusion, we proved the capability of machine learning, and in particular of recurrent neural network, as a tool for assessment and control of a MBE growth process, through RHEED image analysis and growth parameter tracking. The best architecture maintains a classification accuracy of 0.81 specifically during critical phase transitions—a regime where naive and linear extrapolation models proved inadequate. This predictive capability translates to a practical 6–8 s lead time, establishing a viable foundation for expert systems capable of active process control and rapid detection of morphological instabilities. Extending our model with a direct analysis of RHEED image batches without any additional feature extraction step would allow one to identify and track unexpected new phases, and to connect these features to specific areas of RHEED source images. Furthermore, the successful self-evolution of feature

data sets suggests that these lightweight recurrent models could be improved to capture the underlying growth dynamics with sufficient fidelity to serve as state machines, offering a promising pathway toward data-driven digital twins for MBE.

■ ASSOCIATED CONTENT

Data Availability Statement

A broader technical discussion on data collection, net training, and result metrics is given in the [Supporting Information](#). Raw data files, animated prediction movies and additional graphs for selected (N , M) nets can be found in online repository (DOI: [10.5281/zenodo.22082539](https://doi.org/10.5281/zenodo.22082539)).

Supporting Information

The Supporting Information is available free of charge at <https://pubs.acs.org/doi/10.1021/acs.cgd.6c00850>.

S1: Classification mode. Figure. 1. Data classification IRH/RRH phase diagram after manual labeling and modeling with a dense NN classification model. In the inset: typical pattern of a 2D-liquid Ga and 2D-3D transitions. Figure. 2. Confusion matrix for RHEED state classification. S2: DNN training. Figure. 3. (a), depth resolved RMSE for the different prediction nets; (b), training loss progress for net (9,6); (c), RMSE at fixed prediction depth as a function of the total prediction depth M ; (d), depth-resolved RMSE comparison of the same model (18,12) trained with a parametrized shutter function $G_{\text{as}}(t)$ (red) and with a simple digital shutter state (blue). S3: Classification Score. Figure. 4. Accuracy and f1 scores for the full data set and the phase transition limited data subset as a function of the total input depth N (top) and output depth M (bottom) (PDF)

■ AUTHOR INFORMATION

Corresponding Author

Giovanni Drera – Dipartimento di Scienza dei Materiali,
Università di Milanobiccocca, Milano 20126, Italy;
✉ orcid.org/0000-0002-3871-9227;
Email: giovanni.drera@unimib.it

Authors

Stefano Vichi – Dipartimento di Scienza dei Materiali,
Università di Milanobiccocca, Milano 20126, Italy;
✉ orcid.org/0000-0003-4272-4261

Matteo Canciani – Dipartimento di Scienza dei Materiali,
Università di Milanobiccocca, Milano 20126, Italy;
✉ orcid.org/0009-0002-3017-8865

Richard Nötzel – Dipartimento di Scienza dei Materiali,
Università di Milanobiccocca, Milano 20126, Italy;
✉ orcid.org/0000-0003-2672-6363

Stefano Sanguinetti – Dipartimento di Scienza dei Materiali,
Università di Milanobiccocca, Milano 20126, Italy;
✉ orcid.org/0000-0002-4025-2080

Complete contact information is available at:
<https://pubs.acs.org/doi/10.1021/acs.cgd.6c00850>

Notes

The authors declare no competing financial interest.

■ ACKNOWLEDGMENTS

This work was funded by the National Plan for NRRP Complementary Investments (PNC, established with the decree-law 6 May 2021, n. 59, converted by law n. 101 of 2021) in the call for the funding of research initiatives for technologies and innovative trajectories in the health and care sectors (Directorial Decree n. 931 of 06-06-2022) - project n. PNC0000003, Advanced Technologies for Humancentred Medicine (project acronym: ANTHEM). This work reflects only the authors' views and opinions, neither the Ministry for University and Research nor the European Commission can be considered responsible for them.

■ REFERENCES

- (1) Herman, M. A.; Sitter, H. *Molecular beam epitaxy: fundamentals and current status*. Springer Science & Business Media, 2012, vol. 7.
- (2) Pfeiffer, L.; West, K. The role of mbe in recent quantum hall effect physics discoveries. *Phys. E: Low-Dimens. Syst. Nanostructures* **2003**, 20 (1-2), 57–64.
- (3) Tsao, J. Y., *Materials Fundamentals of Molecular Beam Epitaxy*. Academic Press, 2012.
- (4) Okumura, H.; Balakrishnan, K.; Hamaguchi, H.; Koizumi, T.; Chichibu, S.; Nakanishi, T.; Nagatomo, T.; Yoshida, S. Analysis of MBE growth mode for GaN epilayers by RHEED. *J. Cryst. Growth* **1998**, 189189-190190, 364–369.
- (5) McSkimming, B. M.; Wu, F.; Huault, T.; Chaix, C.; Speck, J.S. Plasma Assisted Molecular Beam Epitaxy of GaN with Growth Rates >2.6 m/h. *J. Cryst. Growth* **2017**, 386, 168–174.
- (6) Adelmann, C.S.; Brault, J.; Mula, G.; Daudin, B.; Lymperakis, L.; Neugebauer, J. Gallium adsorption on (0001) GaN surfaces. *Phys. Rev. B* **2003**, 67 (16), 165419.
- (7) Liang, H.; Stanev, V.; Kusne, A. G.; Tsukahara, Y.; Ito, K.; Takahashi, R.; Lippmaa, M.; Takeuchi, I. Application of machine learning to reflection high-energy electron diffraction images for automated structural phase mapping. *Phys. Rev. Mater.* **2022**, 6, 063805.
- (8) Provence, S. R.; Thapa, S.; Paudel, R.; Truttmann, T. K.; Prakash, A.; Jalan, B.; Comes, R. B. Machine learning analysis of perovskite oxides grown by molecular beam epitaxy. *Phys. Rev. Mater.* **2020**, 4, 083807.
- (9) Kaspar, T. C.; Akers, S.; Sprueill, H. W.; Ter-Petrosyan, A. H.; Bilbrey, J. A.; Hopkins, D.; Harilal, A.; Christudasjustus, J.; Gemperline, P.; Comes, R. B. Machine-learningenabled on-the-fly analysis of rheed patterns during thin film deposition by molecular beam epitaxy. *J. Vac. Sci. Technol. A* **2025**, 43 (3), 032702.
- (10) Schaefer, S.; Febba, D.; Egbo, K.; Teeter, G.; Zakutayev, A.; Tellekamp, B. Rapid screening of molecular beam epitaxy conditions for monoclinic (InGa)2O3 alloys. *J. Mater. Chem. A* **2024**, 12, 5508–5519.
- (11) Price, C. C.; Li, Y.; Zhou, G.; Younas, R.; Zeng, S. S.; Scanlon, T. H.; Munro, J. M.; Hinkle, C. L. Predicting and accelerating nanomaterial synthesis using machine learning featurization. *Nano Lett.* **2024**, 24 (46), 14 862–14 867.
- (12) Meng, Z.; Yang, Q.; Yip, P.; Eyink, K.; Taferner, W.; Igelnik, B. Combined use of computational intelligence and materials data for on-line monitoring and control of mbe experiments. *Eng. Appl. Artif. Intell.* **1998**, 11 (5), 587–595.
- (13) Shen, C.; Zhan, W.; Xin, K.; Li, M.; Sun, Z.; Cong, H.; Xu, C.; Tang, J.; Wu, Z.; Xu, B.; Wei, Z.; Xue, C.; Zhao, C.; Wang, Z. Machine-learningassisted and real-timefeedbackcontrolled growth of InAs/GaAs quantum dots. *Nat. Commun.* **2024**, 15 (1), 2724.
- (14) Hu, J.; Zhang, Y.; Sun, M.; Piedra, D.; Chowdhury, N.; Palacios, T. Materials and processing issues in vertical GaN power electronics. *Mater. Sci. Semicond. Process.* **2018**, 78, 75–84.
- (15) Zhong, Y.; Zhang, J.; Wu, S.; Jia, L.; Yang, X.; Liu, Y.; Zhang, Y.; Sun, Q. A review on the GaN-on-Si power electronic devices. *Fundam. Res.* **2022**, 2 (3), 462–475.

- (16) Hidayat, W.; Usman, M. Applications of molecular beam epitaxy in optoelectronic devices: an overview. *Phys. Scr.* **2024**, *99* (11), 112002.
- (17) Vichi, S.; Robin, Y.; Sanguinetti, S.; Pristovsek, M.; Amano, H. Increasing the Luminescence Efficiency of Long-Wavelength (In,Ga)N Quantum Well Structures by Electric Field Engineering Using an (Al,Ga)N Capping Layer. *Phys. Rev. Appl.* **2020**, *14* (2), 024018.
- (18) Jafar, N.; Jiang, J.; Lu, H.; Qasim, M.; Zhang, H. Recent Research on Indium-Gallium-Nitride-Based Light-Emitting Diodes: Growth Conditions and External Quantum Efficiency. *Crystals* **2023**, *13* (12), 1623.
- (19) Zscherp, M.F.; Jentsch, S. A.; Müller, M. J.; Lider, V.; Becker, C.; Chen, L.; Littmann, M.; Meier, F.; Beyer, A.; Hofmann, D. M.; As, D. J.; Klar, P. J.; Volz, K.; Chatterjee, S.; Schörmann, J. Overcoming the Miscibility Gap of GaN/InN in MBE Growth of Cubic In_xGa_{1-x}N. *ACS Appl. Mater. Interfaces* **2023**, *15* (33), 39513–39522.
- (20) Aggarwal, V.; Ramesh, C.; Tyagi, P.; Gautam, S.; Sharma, A.; Husale, S.; Kumar, M.S.; Kushvaha, S. Controlled epitaxial growth of GaN nanostructures on sapphire (11–20) using laser molecular beam epitaxy for photodetector applications. *Mater. Sci. Semicond. Process.* **2021**, *125*, 105631.
- (21) Moseley, M.; Billingsley, D.; Henderson, W.; Trybus, E.; Doolittle, W.A. Transient atomic behavior and surface kinetics of GaN. *J. Appl. Phys.* **2009**, *106* (1), 014905.
- (22) Corrion, A. L.; Wu, F.; Speck, J. S. Growth regimes during homoepitaxial growth of GaN by ammonia molecular beam epitaxy. *J. Appl. Phys.* **2012**, *112* (5), 054903.
- (23) McSkimming, B. M.; Chaix, C.; Speck, J. S. High Active Nitrogen Flux Growth of GaN by Plasma Assisted Molecular Beam Epitaxy. *J. Vac. Sci. Technol., A* **2015**, *33* (5), 05E128.
- (24) Neugebauer, J.; Zywiets, T. K.; Scheffler, M.; Northrup, J. E.; Chen, H.; Feenstra, R. M. Adatom Kinetics On and Below the Surface: The Existence of a New Diffusion Channel. *Phys. Rev. Lett.* **2003**, *90* (5), 056101.
- (25) Mula, G.; Adelman, C.; Moehl, S.; Oullier, J.; Daudin, B. Surfactant Effect of Gallium during Molecularbeam Epitaxy of GaN on AlN (0001). *Phys. Rev. B:Condens. Matter Mater. Phys.* **2001**, *64* (19), 195406.
- (26) Ahmad, H.; Motoki, K.; Clinton, E. A.; Matthews, C. M.; Engel, Z.; Doolittle, W. A. Comprehensive Analysis of Metal Modulated Epitaxial GaN. *ACS Appl. Mater. Interfaces* **2020**, *12* (33), 37693–37712.
- (27) Qayyum, A.; Zeb, S.; Naveed, M. A.; Ghauri, S. A.; Zakaullah, M.; Waheed, A. Diagnostics of nitrogen plasma by trace rare-gas—optical emission spectroscopy. *J. Appl. Phys.* **2005**, *98* (10), 103303.
- (28) Schulz, C.; Schmidt, T.; Flege, J. I.; Berner, N.; Tessarek, C.; Hommel, D.; Falta, J. Oxide removal from GaN(0001) surfaces. *Phys. Status Solidi (c)* **2009**, *6*, S305–S308.
- (29) Canciani, M.; Vichi, S.; Koplak, O.; Bietti, S.; Sanguinetti, S. In situ control of GaN growth rate in nitrogen-limited regime. *J. Vac. Sci. Technol. A* **2025**, *43*, 032704.
- (30) Cho, K.; van Merriënboer, B.; Bahdanau, D.; Bengio, Y. On the properties of neural machine translation: Encoderdecoder approaches. *arXiv* **2014**, arXiv.1409.1259.