A trained Physics-Informed Neural Networks (PINNs) method for phase-field model in Allen-Cahn framework

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1. Introduction

The Asaro-Tiller-Grinfeld (ATG) instability, driven by misfit strain in thin films, significantly impacts the stability and performance of semiconductor devices[1]. Traditional numerical models for ATG instability are computationally expensive and limited in predictive accuracy. This study integrates Physics-Informed Neural Networks (PINNs) with a phase-field model to predict and analyze ATG instability. PINNs embed physical laws into deep learning, significantly reducing computational time while improving accuracy. [2]

2. Methodology

We reformulate the governing equations of ATG instability into a residual-based PINN framework. The surface chemical potential, interface motion, and phase-field evolution are encoded into the loss function, ensuring physical consistency. The PINN-enhanced phase-field model is implemented using the Allen-Cahn framework, enabling efficient prediction of instability thresholds and morphology evolution, as shown in Figure 1.

The phase-field evolution is governed by the Allen-Cahn equation[3]:

$$\frac{\partial \phi_\alpha}{\partial t} = -\frac{1}{\varepsilon \widetilde{N}} \sum_{\beta \neq \alpha}^{\overline{N}} M_{\alpha\beta} \left(\frac{\delta F}{\delta \phi_\alpha} - \frac{\delta F}{\delta \phi_\beta} \right),$$

where ϕ_α is the phase-field variable, F is the free energy, and $M_{\alpha\beta}$ is the mobility coefficient.

The PINN loss function is defined as:

$$\mathcal{L}_{total} = \lambda_1 \mathcal{L}_\mu + \lambda_2 \mathcal{L}_{v_n} + \lambda_3 \mathcal{L}_h + \lambda_4 \mathcal{L}_\omega + \lambda_5 \mathcal{L}_\phi + \lambda_6 \mathcal{L}_\sigma,$$

where $\mathcal{L}_\mu$, $\mathcal{L}_{v_n}$, $\mathcal{L}_h$, $\mathcal{L}_\omega$, $\mathcal{L}_\phi$, and $\mathcal{L}_\sigma$ are the residuals for surface chemical potential, interface motion, interface height, dispersion relation, phase-field evolution, and mechanical equilibrium, respectively.

Physics-Informed Neural Networks (PINNs) approximate the solutions by minimizing residuals of the governing equations.

3. Results and discussion

The PINN method is nearly 10× faster than traditional numerical solvers.Traditional methods require extensive iterative solving (120-140 sec per simulation).PINNs leverage physics constraints and deep learning to predict results in 10 sec. Traditional methods show higher error rates (7.8-8.9 percent) due to numerical approximations. The PINN model has a much lower error (2.0-2.4 percent), indicating better predictive capability. Traditional numerical solvers struggle with long-wavelength perturbation predictions, leading to high instability errors (ca. 15 percent). PINN models significantly reduce stability prediction errors (ca.5 percent), meaning better handling of nonlinear effects,as shown in Figure 2.

This comparison demonstrates that PINNs offer a game-changing alternative to traditional numerical simulations for fast, accurate, and efficient ATG instability analysis. We utilized the Physics-Informed Neural Network (PINN) algorithm to investigate and determine the maximum critical stress that a growing film can sustain under varying values of the parameter ε. By leveraging the PINN framework, which integrates physical laws into the neural network's training process, we were able to accurately model the stress distribution and evolution over time.as shown in Figure 3.

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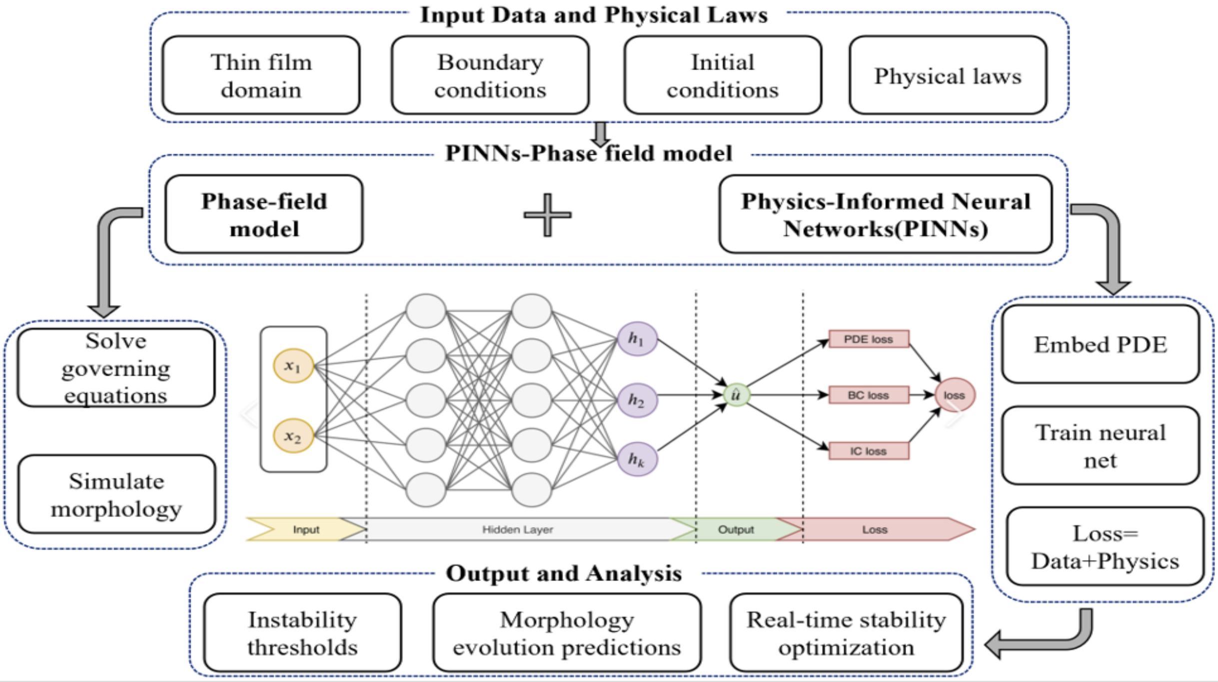

Fig. 1: The framework of Physics-informed neural network combined Phase-field model.

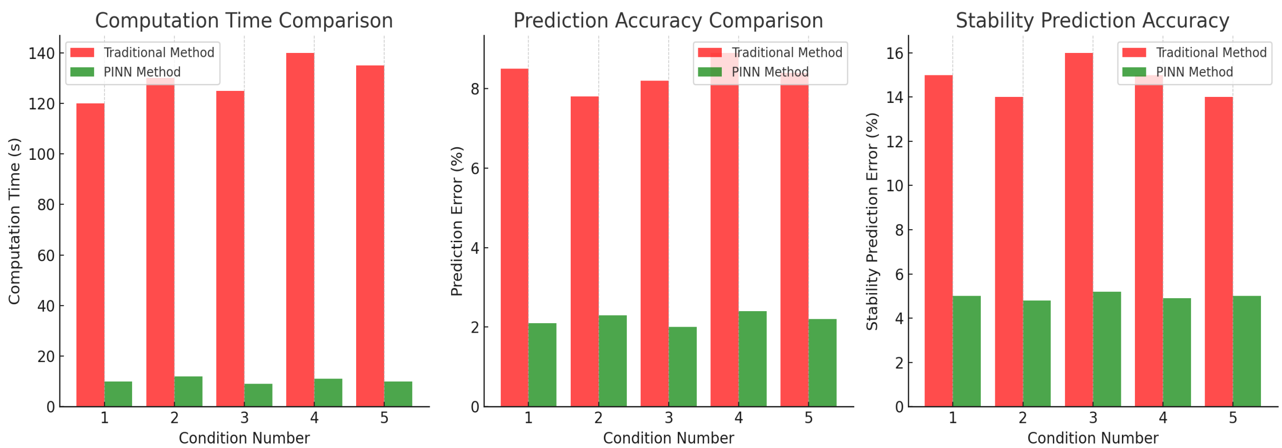

Fig. 2: Comparison of the PINN method with classic Phase-field model.

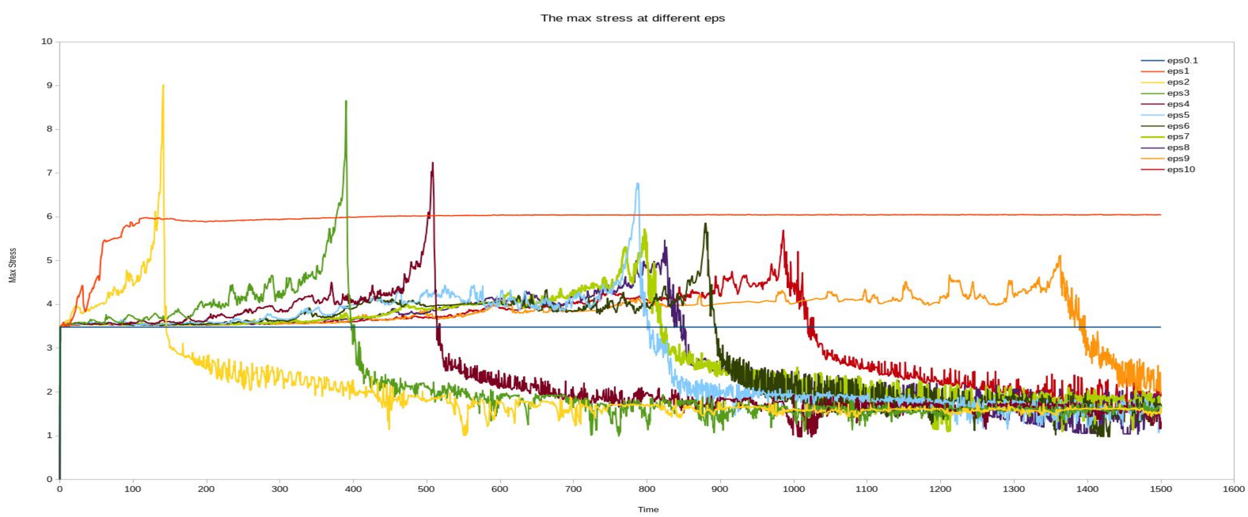

Fig. 3: The variation of the stress with time at different eps.