Hybrid Modeling of TCAD and AI for Semiconductor Design

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Data-driven and physics-based models are complementary to each other in solving scientific or engineering problems, as shown in Table I. As such, merging machine learning (ML) or artificial intelligence (AI) and simulation has received growing interest to completely exploit their combined potential [1]–[4]. Here we concentrate on application of hybrid modeling of ML/AI and TCAD simulation to develop and optimize semiconductor process technologies and devices. Fig. 1(a) shows a schematic of AI-based emulator to mimic the TCAD process and device simulation for real-time prediction. First, to generate doping profiles as shown in Fig.1(c), AI-learned process emulator uses a tailored convolutional neural network. Secondly, for a device emulator we adopted a recurrent neural network structure which is specially designed to learn sequential data, because current vs. voltage (I-V) curves can be regarded as sequential data and current values of neighboring voltage points are highly correlated. To improve a prediction accuracy for I-V, trans-conductance characteristics is considered simultaneously while training the AI model. Fig. 1(b) shows that the emulator reproduces the relationship between drain current and gate voltage and drain voltage, and cross-section of device with current density contours at different drain bias is as shown in Fig. 1(d). Fig. 2 illustrate a hybrid approach of ML and physical model to accurately describe the etch processes for deep trench isolation with considering features such as type of process scheme, equipment information that physical simulator cannot take into account. Sequence-to-sequence ML model is used as a baseline model since both inputs and outputs are sequential data in time as in Fig. 2(a). Fig. 2(b) shows how the baseline model works and that the predicted profile at a final time step (denoted as t_{final}) well match actual process results (red dashed line). It turns out, however, that the baseline AI model cannot properly predict profile evolution as the time progresses (t_1~ t_5). A physical compact model is used to impose a physics-based topology constraint on the baseline model to learn causality between each steps. Fig. 2(c) demonstrates that incorporating such physical insights help AI model predict correctly profile evolution at intermediate steps.

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Table 1: Comparison of Pros (◎) and Cons (◌) between Physics-based Model and Data-driven Model

Symbol		Physics-based Model	Data-driven Model
Data Cost		◎	◌
Accuracy	Extrapolation	◎	○
	Interpolation	○	◎
Inverse Optimization		○	◎
Interpretability		◎	◌
Prediction Time		◌	◎

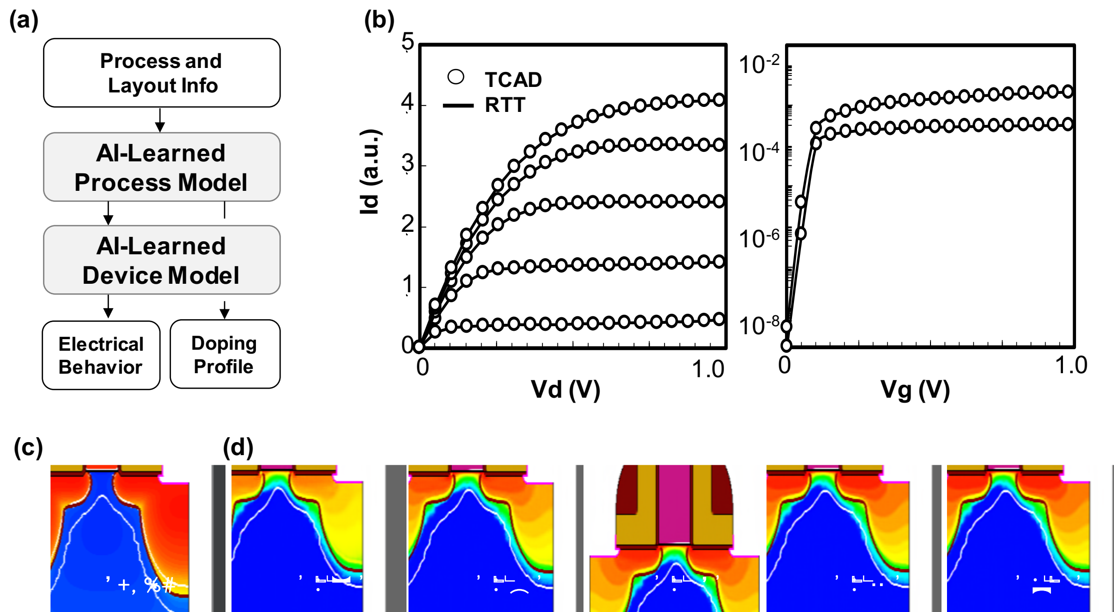

Figure 1: (a) a schematic of AI-based emulator for real-time prediction. (b) current-voltage characteristics between TCAD and AI-emulator shows good agreement with each other. (c) AI-emulator generated doping profiles and (d) cross-section of device with current density contours at different drain bias

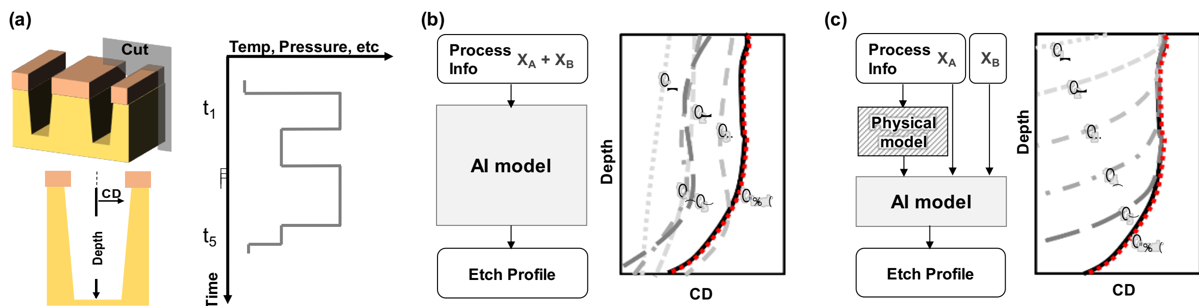

Figure 2: (a) a schematic of deep trench isolation (DTI), and input example for DIT etching process such as type of gas, temperature, pressure, etc. (b) predicted profile with the baseline model : the DTI is vertically etched down to bottom layer in the beginning of processes. (c) The unphysical behavior is fixed with hybrid modeling of physical and AI model.

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