# RL-Based Diode Design Environment Analysis

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## Project Goal

This project aims to automate semiconductor diode design using reinforcement learning (RL). The system teaches an AI agent to generate complete DEVSIM (semiconductor device simulation) scripts by learning the proper sequence of device fabrication and simulation setup steps.

## Core Objectives:

Automated Script Generation: Replace manual DEVSIM scripting with AI-generated code
Design Optimization: Learn optimal doping concentrations (Na, Nd) and fabrication sequences
Process Learning: Understand dependencies between fabrication steps
Performance Optimization: Maximize forward current while minimizing reverse leakage

## Methodology

### 1. Reinforcement Learning Framework

Environment: Custom Gymnasium environment (DiodeDesignEnv)
Agent: Makes decisions about which fabrication step to perform next
State Space: 18-dimensional observation vector containing:

15 boolean flags for completed fabrication steps
2 normalized doping parameters (Na, Nd)
1 normalized step counter

Action Space: 15 discrete actions corresponding to fabrication steps

### 2. Fabrication Process Modeling

The system models a complete diode fabrication workflow:

```
INIT_MESH → DEFINE_GEOMETRY → DEFINE_REGIONS → DEFINE_CONTACTS
   ↓
FINALIZE_MESH → CREATE_DEVICE → SET_MATERIAL_PARAMS
   ↓
DEFINE_P_DOPING → DEFINE_N_DOPING → DEFINE_NET_DOPING
   ↓
DEFINE_VARIABLES → SETUP_PHYSICS → SETUP_EQUATIONS
   ↓
SETUP_CONTACT_BC → FINALIZE_SETUP_RUN_TEST
```

### 3. Code Generation Strategy

Dynamic Script Building: Each action generates specific DEVSIM Python code
Dependency Checking: Enforces realistic fabrication constraints
Parameter Integration: Incorporates design parameters into generated code
Execution Validation: Can execute generated scripts for immediate feedback

### 4. Reward System

Multi-objective optimization considering:

Forward Current (If): Higher is better (eg. target: ≥1e-4 A)
Reverse Leakage (Ir): Lower is better (eg. target: ≤1e-9 A)

Current Ratio: Maximizes If/Ir ratio
Step Efficiency: Penalizes unnecessary steps
Process Violations: Heavy penalties for invalid sequences

## The Outcome

The final output of this project is a trained RL agent that has learned an optimal policy for designing a specific type of semiconductor device (like the proof-of-concept 1D diode).

When this trained agent is run, it will:

Autonomously select a sequence of design steps and their parameters.
Generate a complete, valid Python script for the DEVSIM simulator.
The generated script will define a device that is optimized for high-performance characteristics (e.g., a high forward-to-reverse current ratio), as defined by the project's reward function.
Ultimately, this creates a system that can automate and accelerate the discovery of novel and efficient semiconductor device designs.