Characteristic Determination for Solid State Devices with Evolutionary Computation

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Abstract

In this paper, we develop a new optimization framework that consists of the extended compact genetic algorithm (ECGA) and split-on-demand (SoD), an adaptive discretization technique, to tackle the characteristic determination problem for solid state devices. Because most decision variables of characteristic determination problems are real numbers due to the modeling of physical phenomena, and ECGA is designed for handling discrete-type problems, a specific mechanism to transform the variable types of the two ends is in order. In the proposed framework, ECGA is used as a back-end optimization engine, and SoD is adopted as the interface between the engine and the problem. Moreover, instead of one mathematical model with various parameters, characteristic determination is in fact a set of problems of which the mathematical formulations may be very different. Therefore, in this study, we employ the proposed framework on three study cases to demonstrate that the technique proposed in the domain of evolutionary computation can provide not only the high quality optimization results but also the flexibility to handle problems of different formulations.

1 Introduction

The realization of modern computing equipment, which vastly contributes to all the fields related to computation, relies on the advance and development of the integrated circuit (IC) [1, 2]. One the most fundamental and important element in the integrated circuit is the solid state device [3, 4], for example, the bipolar junction transistor (BJT) [4], the metal-oxide-semiconductor field-effect transistor (MOSFET) [5], the thin-film transistor (TFT) [6], and the like. The solid state device is the basic building blocks for the integrated circuit. The quality and properties of the solid state device are critical to the integrated circuit and are therefore critical to the computer systems which are built up on the integrated circuit. Hence, the development of solid state devices plays an essential role in modern computation from a fundamental perspective.

One of the key issues in developing the solid state device is to determine crucial characteristics for the observed physical phenomena [7, 8]. Different structures, materials, or fabrication processes can make the produced device to possess different properties. In order to gain understandings of how the device operates and to improve current devices or invent new devices, characteristic determination has to be properly conducted. Unlike those problems, which is composed of one mathematical model with various parameters, often tackled in the computation related disciplines, characteristic determination is in fact a variety of problems of which

the mathematical formulations may be very different thanks to the different underlying physical phenomena. Thus, although certain optimization techniques might be utilized to handle some characteristic determination problems, it is very difficult to employ a single method to determine parameters coming from dissimilar physical models.

Given the importance and difficulty of the characteristic determination problem for solid state devices, researchers and developers oftentimes take two approaches. One is to make a lot of efforts to adopt a traditional optimization method for every encountered physical model. The other is to manually determine the characteristics. Manual determination usually involves several person-weeks or even person-months to handle only a few problems. However, the methods proposed in evolutionary computation, such as genetic algorithms (GA) [9, 10, 11, 12], offer an alternative approach thanks to their flexibility. In order to speed up the development of solid state devices as well as to relocate the manpower for better use, we develop a new framework based on the techniques in evolutionary computation.

Particularly, in the present work, we adopt the extended compact genetic algorithm (ECGA) [13] as the back-end optimization engine and the split-on-demand (SoD) technique [14], an adaptive discretization method, as the interface between ECGA and the characteristic determination problem. We employ the proposed framework to tackle three different characteristic determination problems encountered while conducting research on thin-film transistors. The numerical results we obtained for determining the characteristics on the three study cases demonstrate that the proposed framework can handle problems of different natures and deliver high quality solutions in an efficient manner.

The remainder of the paper is organized as follows. In section 2, the idea, integration, and workflow of the real-coded ECGA, which is composed of ECGA and SoD, are described in detail. In section 3, we employ the proposed framework to tackle three characteristic determination problems of different natures. Finally, section 4 gives a summary and draws conclusions.

2   The Real-Coded ECGA

The real-coded ECGA is a new optimization framework, composed of the extended compact genetic algorithm [13] and split-on-demand (SoD) [14], proposed in the study. In this section, we will first give a brief review of ECGA, then describe how SoD discretizes real numbers for ECGA, and introduce the integration of ECGA and SoD.

2.1   A Brief Review of ECGA

The major difference between ECGA and traditional genetic algorithms is that ECGA is one of the estimation of distribution algorithms (EDAs) [15, 16], which use probability models to describe populations and replace the crossover operator with sampling procedures. There are two main assertions behind the concept of ECGA. First, learning a "good" probability distribution is equivalent to learning linkage. Second, the "goodness" of a probability distribution is based on how much space is needed to store the population as well as the distribution.

As a precursor of ECGA, the compact GA (cGA) [17] revealed that the population in genetic algorithms can be represented as a probability distribution, and the role of crossover can be played by sampling the model. Thus, finding the optimal solution in cGA is equivalent to finding the optimal probability distribution. ECGA extends the probability model in cGA to the marginal product model (MPM). MPMs are similar to the models of the cGA and PBIL [18], except that they can represent a probability distribution over more than one gene at a time.

The goal of ECGA is to find "good" distributions, but how do we define the criterion of the quality of a distribution? The answer is the idea of Occam's Razor [19]:

By reliance on Occam's Razor, good distributions are those under which the representation of the distribution using the current encoding, along with the representation of the population compressed under that distribution, is minimal.

This idea leads to the definition of the *minimum description length* (MDL) [20]. Following the definition, we can use MDL on MPMs and define the model complexity and compressed population complexity of a probability distribution:

$$\text{Model Complexity} = \log_2 N \sum_{i=1}^{m} 2^{s_i} \, , \tag{1}$$

and

$$\begin{aligned}\text{Compressed Population Complexity} \\ = N \sum_{i=1}^{m} \sum_{p} -p \log_2 p \, . \end{aligned} \tag{2}$$

In these formulas, m is the number of subsets, s_i the size of the ith subset, p is the probability of a pattern in the ith subset, and N is the population size. The combined complexity is the summation of model complexity and compressed population complexity.

In each generation, after selection, ECGA searches for good MPMs based on their combined complexity to model the current population. The MPM with the minimal combined complexity is the very model to use. By sampling the obtained model, the offspring population is created, and the evolutionary process for optimization is repeated iteratively.

2.2 Split on Demand for Discretization

ECGA is designed for handling problems in the discrete domain. In order to employ ECGA to tackle problems in the continuous domain, certain mechanism is need to transform the type of variables. In this work, we adopt an adaptive discretization technique, called split-on-demand (SoD) [14], to encode the individuals as real vectors into the ones as binary strings such that ECGA can accomplish the optimization task without significant modifications.

The main idea of SoD is to split the interval where we demand to obtain more information in order to build a more accurate probabilistic model for the region. There are two parameters for SoD: the *split rate*, γ, and the *split rate decay*, ϵ. γ is used to determine whether or not an interval should be split. Assuming that the population size is N, if an interval contains more than or equal to $N \times \gamma$ individuals, this interval should be split into two small intervals at a random position. By adjusting the split rate, we can control the accuracy of the probabilistic model and the size of code table. Figure 1 illustrates a splitting process under different γ. In Figure 1(a), $\gamma = 0.5$ and the search space is split into three intervals. In Figure 1(b), because γ gets smaller, the search space is split into more intervals.

Most good optimization algorithms consist of two elements: exploitation and exploration. In the proposed framework, we control the degree of exploitation vs. the degree of exploration by adjusting the split rate γ. We use a decreasing factor: ϵ, where $0 < \epsilon < 1$ to manipulate γ. At the early stage of search, we need more exploration than exploitation. γ is set to 0.5, which means that one dimension of the search space will be split into only two or three intervals. As the search process goes, exploitation is more and more important. We multiply γ with ϵ at each generation to make it gradually smaller and smaller, and the MPM model is more and more accurate for the regions filled with individuals. Finally, Algorithm 1 shows the SoD pseudo code.

(a) Population distribution and 2 split positions at generation 1. $\gamma = 0.5$. $10 \times \gamma = 5$.

(b) Population distribution and 4 split positions at generation 10. $\gamma = 0.4$. $10 \times \gamma = 4$.

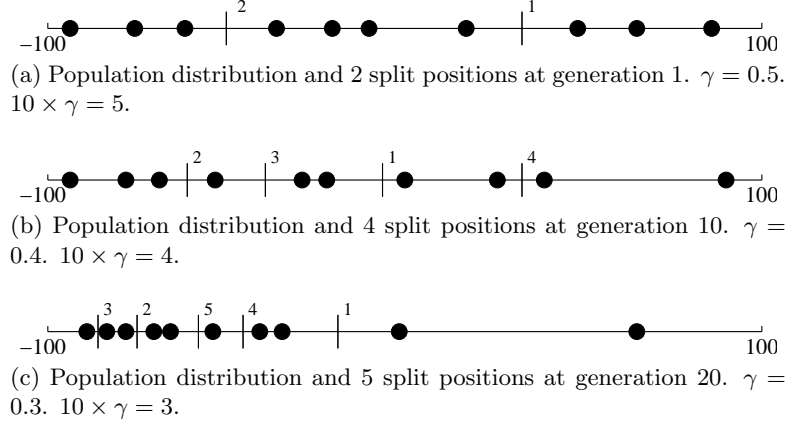(c) Population distribution and 5 split positions at generation 20. $\gamma = 0.3$. $10 \times \gamma = 3$.

Figure 1: Populations and possible split positions (vertical lines). The numbers close to the positions are the order in which the positions are decided.

2.3 ECGA with SoD

With the help of SoD, the real-coded ECGA (rECGA) can now handle problems in the continuous domain. The population in rECGA is represented in two forms: real vectors and binary strings. In the evaluation and selection phases, the population is in the form of real vectors. In the modeling and crossover phases, the population is in the binary-string form. SoD transforms real vectors into binary strings, and binary strings are converted back to real vectors by using random sampling. For example, if the code of an individual is 11 in binary, and the interval for the code 11 is $[-50, 0]$, the value is uniformly randomly sampled in the interval $[-50, 0]$. Finally, the integration of ECGA and SoD, the proposed frameworkr, is shown in Algorithm 2.

Algorithm 1 Pseudo code for SoD.

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procedure SPLIT-ON-DEMAND
    Split(*lower_bound*, *upper_bound*)
    $\gamma \leftarrow \gamma \times \epsilon$
end procedure

procedure SPLIT(ℓ, u)
    $m \leftarrow \text{random}[\ell, u]$
    $N_\ell \leftarrow$ number of individuals in $[\ell, m]$
    $N_u \leftarrow$ number of individuals in $[m, u]$
    if $N_\ell \geq N \times \gamma$ **then**
        Split(ℓ, m)
    else
        Add a code for the range $[\ell, m]$
    end if
    if $N_u \geq N \times \gamma$ **then**
        Split(m, u)
    else
        Add a code for the range $[m, u]$
    end if
end procedure

Algorithm 2 Pseudo code for the real-coded ECGA.
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  procedure RECGA
      $Gen \leftarrow 1$
      Initialize N individuals of real-numbers at random
      while $Gen \leq Gen_{max}$ **do**
          Evaluate the population of size N
          Perform tournament selection of size S
          Use SoD to produce the code table
          Encode the population by using the code table
          Model the encoded population with MPM search
          Perform crossover with the given MPM model
          Generate the offspring with the code table
          $Gen \leftarrow Gen + 1$
      end while
  end procedure
___

3   Case Study

In the previous section, we proposed a new optimization framework in order to handle the characteristic determination problem for solid state devices. In this section, we apply the proposed framework to tackle three characteristic determination problems which we encountered while conducting research on developing thin-film transistors (TFT). The first one is to determine the quality parameters of the poly-Si thin-film under the normal condition, and the second one deals with different materials and fabrication processes under high gate bias. Finally, the third case is to determine the frequency response property of the solid state device.
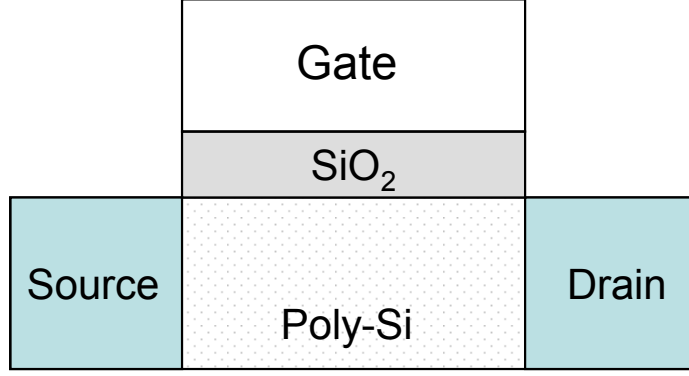
3.1   Conventional TFT

A conventional poly-Si thin-film transistor, as shown in Figure 2(a), is composed of three terminals: gate, source, and drain. When the transistor is turned on, electrons will transport from source to drain through the poly-Si area (the dotted area in the figure), and a high-conducting channel will be formed on the top of this poly-Si area, as shown in Figure 2(b). The poly-Si area can exhibit a wide range of thin-film qualities. For a high quality poly-Si film, electrons can easily transport through it. As a result, the transistor can provide a large conduction current. For a low quality poly-Si thin-film, on the contrary, the electrical conductivity is low and the transistor output current is also reduced. Therefore, controlling the quality of the poly-Si film is essential to the creation and production of high-performance transistors. In addition to the output current, the quality of the poly-Si thin-film in the device is also a key issue to design the fabrication process and to develop the physical model as well as the SPICE model.

    To characterize the poly-Si thin-film quality, the *defect state distribution*, $N(E)$, as follows is usually utilized.

$$N(E) = \frac{N_d}{\sqrt{2\pi}S_d} \exp\left(-\frac{(E - E_{td})^2}{2S_d^2}\right) + N_t \exp\left(-\frac{E_c - E}{E_{tt}}\right) , \qquad (3)$$

where parameters N_d, S_d, E_{td}, N_t, and E_{tt} represent the properties of TFT. However, in practice, these parameters are not available and cannot be directly measured. Instead, these parameters have to be determined by measuring the observable experimental data and matching the equation

$$q \int_{E_c - E_{amax}}^{E_c - E_a} N(E)dE = C_{ox}\left(V_G - V_{fb} - \phi_s\right) , \qquad (4)$$

(a) Structure of poly-Si TFT.
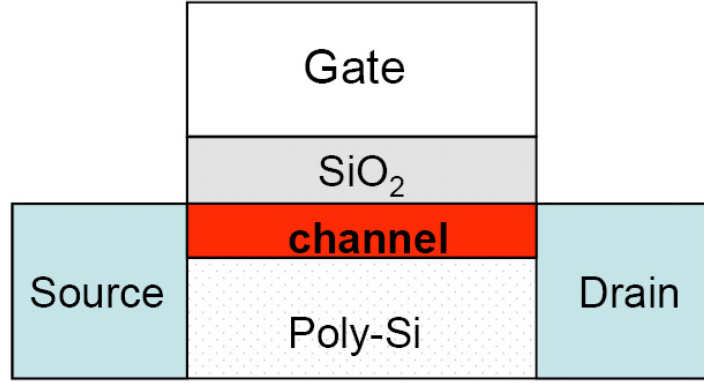
(b) High-conducting channel for TFT.

Figure 2: Structure and the high-conducting channel formed for the conventional poly-Si TFT.

where $q = 1.6 \times 10^{-19}$, $C_{ox} = 7 \times 10^{-8}$, $E_c = 1.2$ are constants, and E_a, E_{amax}, V_G, V_{fb}, and ϕ_s are obtained from the experimental observation, to establish the relationship between the quality measurements (N_d, S_d, E_{td}, N_t, E_{tt}) and the observed outcomes (E_a, E_{amax}, V_G, V_{fb}, ϕ_s). After calculating the integral in Equation (4), we obtain

$$\frac{C_{ox}V_G}{q} = \left[\frac{-N_d S_d}{2} \operatorname{Erf}\left(\frac{E_{td} - E}{\sqrt{2}S_d} \right) + N_t E_{tt} \exp\left(\frac{E - E_c}{E_{tt}} \right) \right] \Bigg|_{E_c - 0.6}^{E_c - E_a}, \tag{5}$$

where Erf($\cdot$) is the error function.

The characteristic determination problem in this case is to find the values of $N_d, S_d, E_{td}, N_t, E_{tt}$ according to the given set of measured values of E_a vs. V_G such that Equation (5) can be matched. We measured the value of E_a for $V_G = 0, \ldots, 10.0$ for every 0.1, and obtained 101 pairs of (E_a, V_G). The objective value for matching Equation (5) is defined as the sum of the absolute value of the differences between the calculated results and the 101 pairs of experimental data. Moreover, the ranges of the parameter can be decided according to physical laws. In this case, the ranges for the five parameters are

- N_d: 10^9–10^{15};

- S_d: 10^{-2}–10^0;
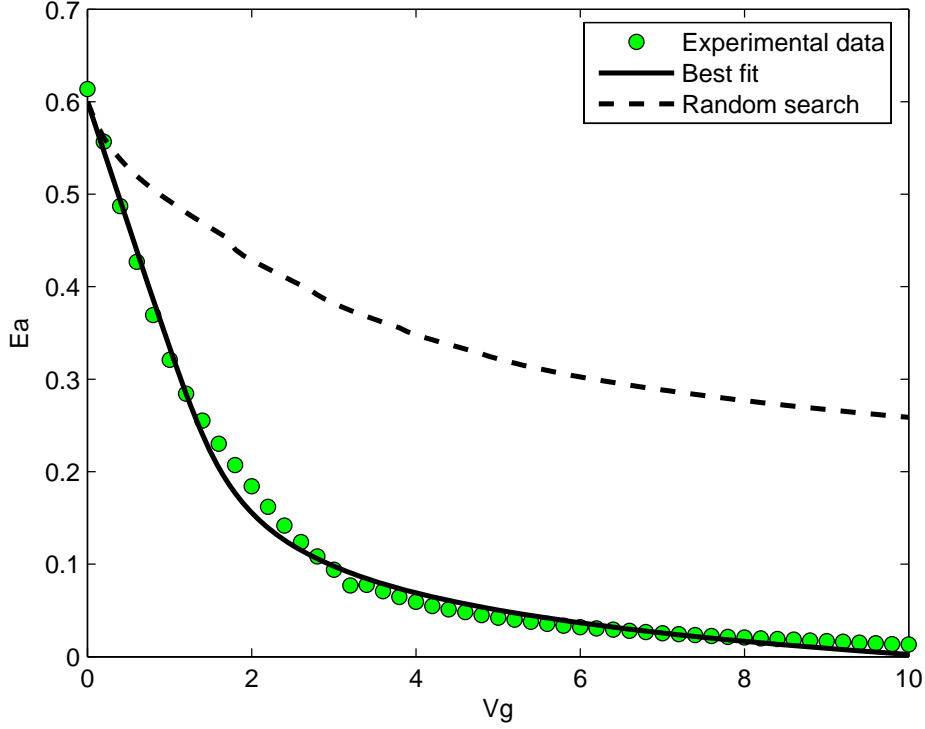
- E_{td}: 0.5–0.7;

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Figure 3: Experimental data and the match results for study case I.

- N_t: 10^{11}–10^{17};

- E_{tt}: 0.05–1.0.

We ran rECGA with 250 individuals for 25 generations. Detailed parameters of rECGA are shown in Table 1. In the 50 independent trials, the curve generated from the best solutions is shown as the solid line in Figure 3. To simply verify that the results we obtained are not merely "lucky shots", we also conducted the pure random search for $250 \times 25 \times 50$ function evaluations. The result for the random search is shown as a dashed line in the figure. As we can see in the figure, the curve generated the pure random search goes very far from experimental data. As a side note, the curve of a similar matching quality can also be manually obtained for about three to five person-days, while the proposed framework takes only minutes to finish all the 50 trials.

Parameter	Value
Population size (N)	250
Tournament size (S)	8
Number of generation (Gen_{max})	25
Crossover probability	0.975
Initial split rate (γ)	0.5
Split rate decay (ϵ)	0.995

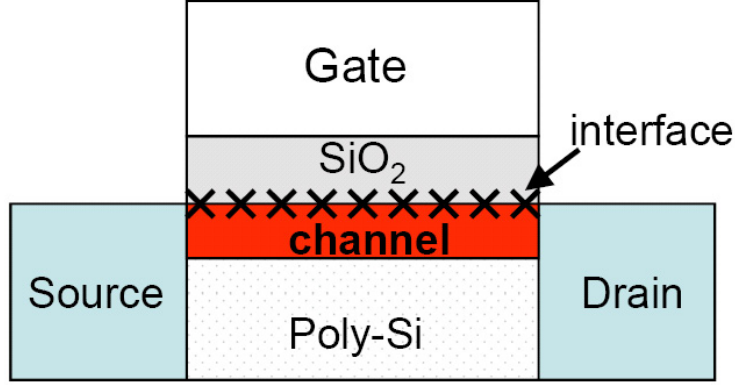Table 1: Parameters adopted in the real-coded ECGA for handling the three study cases.

Figure 4: TFT under high gate bias.

3.2 TFT under High Gate Bias

When the transistors are operated under high gate bias, it is reported that the interface, as shown in Figure 4, between the poly-Si and the gate insulator also has great influence on the output current. As a consequence, to determine the property of TFTs under high gate bias, an interface-state distribution is inserted into $N(E)$ to model the overall defect quality:

$$N(E) = \frac{N_d}{\sqrt{2\pi}S_d} \exp\left(-\frac{(E - E_{td})^2}{2S_d^2}\right) + N_t \exp\left(-\frac{E_c - E}{E_{tt}}\right) + N_i \exp\left(-\frac{E_c - E}{E_{it}}\right) , \quad (6)$$

where N_i and E_{it} are two more fitting parameters for the interface-state distribution. The ranges of N_i and E_{it} are

- N_i: 10^{11}–10^{20};

- E_{it}: 0.05–1.0.

In this study case, we determine the quality parameters for four kinds of TFTs: ELA [21], FLA [22], SSL [23], and SPC [24]. There are several instances for each kind of TFT, and for simplicity in the present work, we choose only one or two instances to perform the computation. Similar to the previous study case, the values of the quality parameters can be obtained by fitting the experimental data to Equation (6). The parameters for rECGA are identical to those used for case I, which is shown in Table 1. The curves generated by the best solutions in the 50 independent trials are shown as solid lines in Figure 5, and the best results obtained by the pure random search are shown as dashed lines. As we can observe in the figures, the pure random search can only match the first data point in all cases, while the proposed framework can provide high quality matching curves. Furthermore, these problem instances cannot be easily handled by human manipulation. We merely succeeded in manually matching a few problem instances for several person-weeks.

3.3 Frequency Response

The previous-addressed poly-Si thin-film quality and the interface quality also influence the frequency response of transistors. Since in circuitry, transistors may be operated under various frequencies, the frequency response is a very important property to determine the fabrication process, to determine the device model, and to determine the circuit design. In poly-Si TFTs, the frequency response is characterized through the capacitance measurement. As indicated in Figure 6(a), the gate/SiO$_2$/poly-Si structure can be expressed by the equivalent circuit depicted
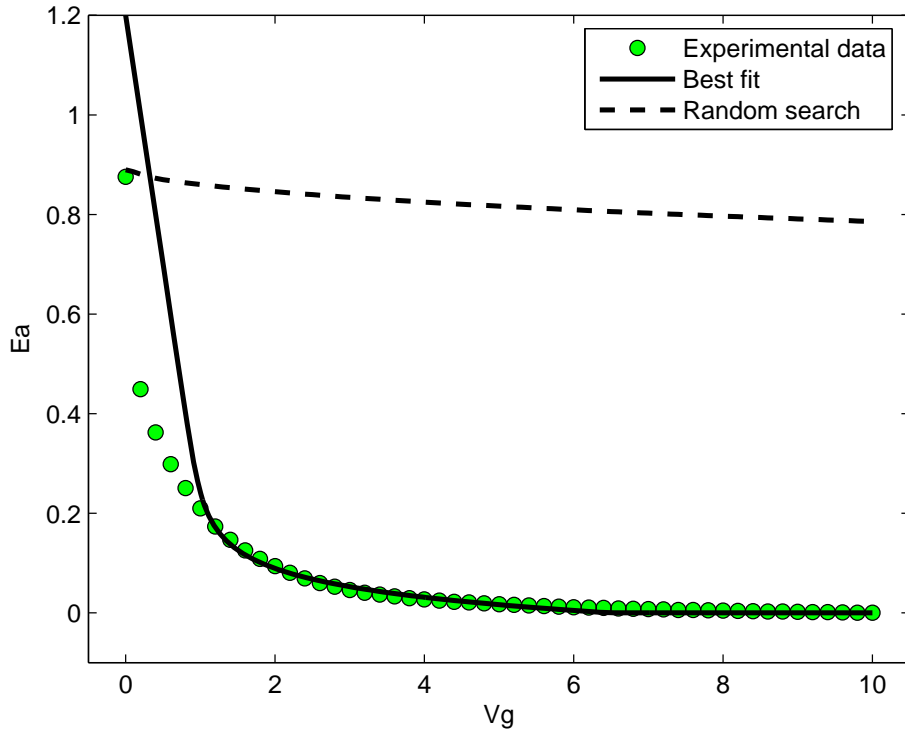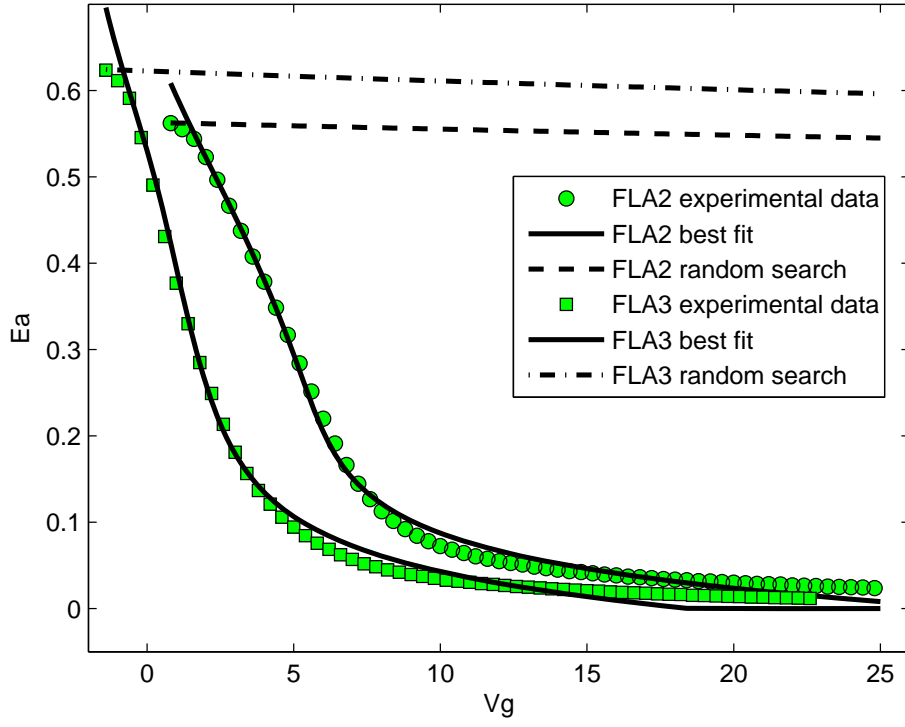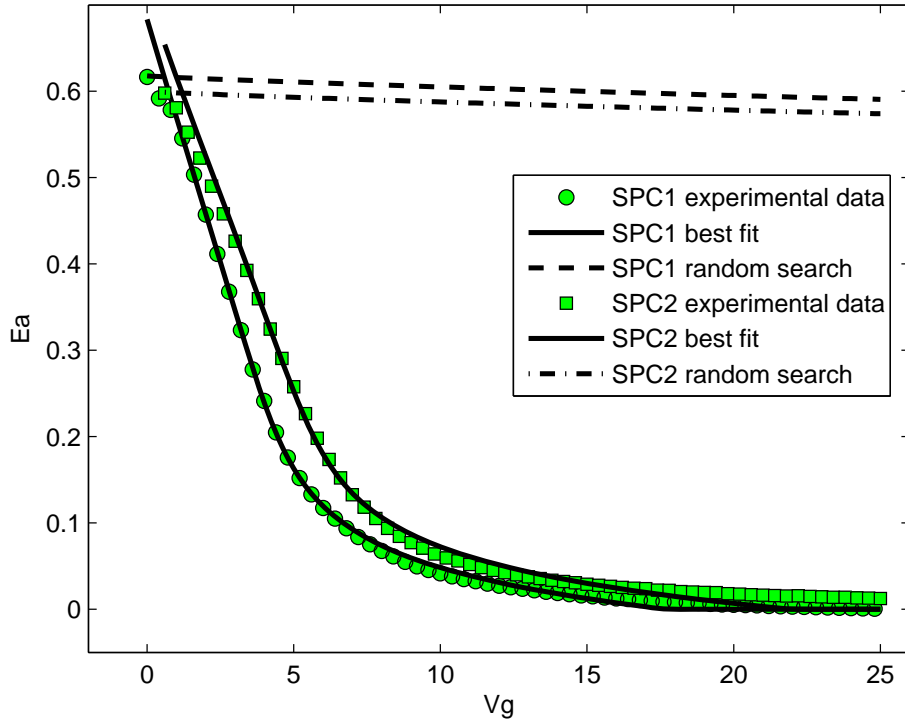
(a) ELA
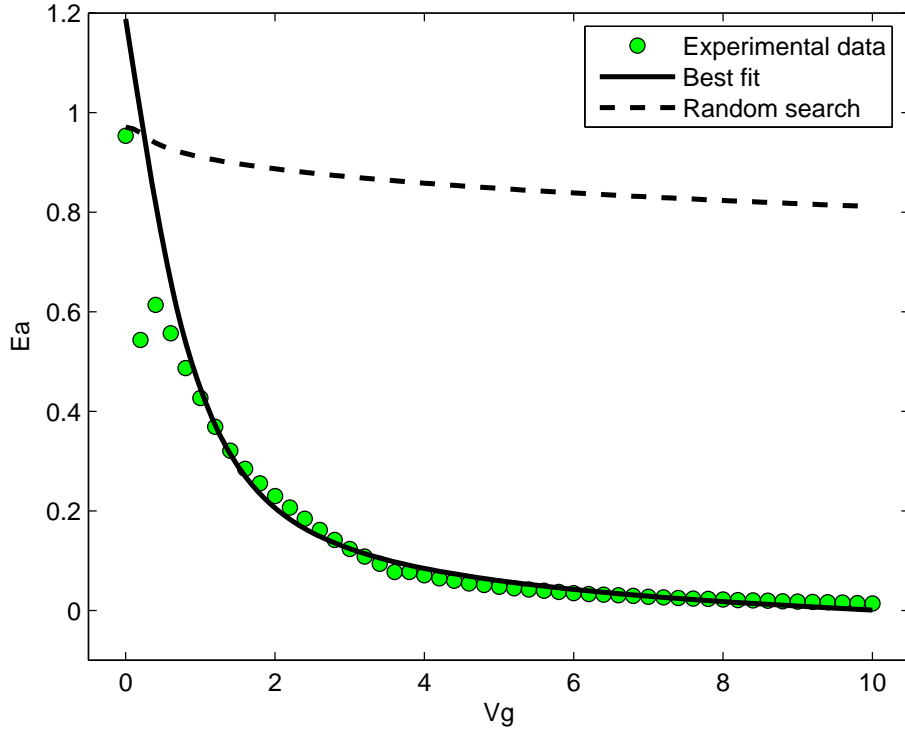
(b) SSL

Figure 5: Experimental data and the match results for study case II. ELA, SSL, FLA, and SPC are four different kinds of TFTs.
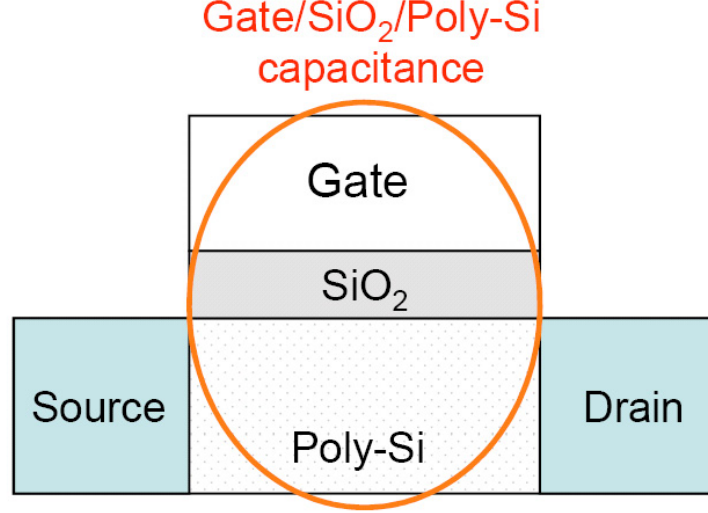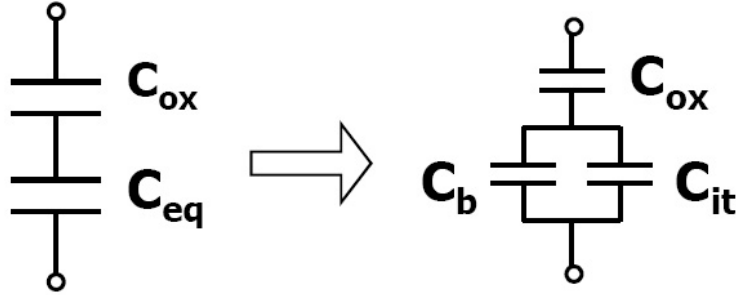
(c) FLA

(d) SPC

Figure 5: Experimental data and the match results for study case II. ELA, SSL, FLA, and SPC are four different kinds of TFTs.

(a) Structure of gate/SiO$_2$/poly-Si.

(b) Equivalent circuit for the structure.

Figure 6: Structure of gate/SiO$_2$/poly-Si and its equivalent circuit.

in Figure 6(b). That is, the total effective capacitance is the series of the oxide capacitance C_{ox} and the equivalent parasitic capacitance C_{eq}. The equivalent parasitic capacitance C_{eq} is the shunt of the bulk capacitance C_b and the interface capacitance C_{it}. Generally, C_{ox} is a constant, which is independent of gate bias or frequency, while C_b and C_{it} have a dependence on frequencies according to the following equation

$$C_{eq} = C_{it} + C_b = qD_{it}\frac{\tan^{-1}(\omega\tau_{it})}{\omega\tau_{it}} + qD_s\frac{\tan^{-1}(\omega\tau_s)}{\omega\tau_s} \ , \tag{7}$$

where ω is $2\pi f$, and f is the frequency. D_{it} and τ_{it} are independent of frequencies, but depend on gate biases. D_s and τ_s are independent of both frequencies and gate biases, since the frequency and gate bias should not strongly influence the bulk properties.

As the previous two study cases, the frequency response parameters (D_{it}, τ_{it}, D_s, τ_s) cannot be directly measured, either. As a result, we measure C_{eq} under various gate biases and frequencies and determine the frequency response parameters according to the observed experimental data. The frequency response of C_{eq} under different gate biases are shown in Figure 7. The values of gate biases and frequencies we used to obtained the experimental data are

- Gate biases: -1.3, -1.4, -1.5, -1.6, -1.7, -1.8, -1.9, -2.0, -2.1, -2.2;

- Frequencies: 1×10^4, 3×10^4, 5×10^4, 1×10^5, 3×10^5, 5×10^5, 1×10^6.

There are totally 70 values for C_{eq} under the combinations of gate biases and frequencies measured. We used these experimental data to calculate C_{eq} according to Equation (7). As shown
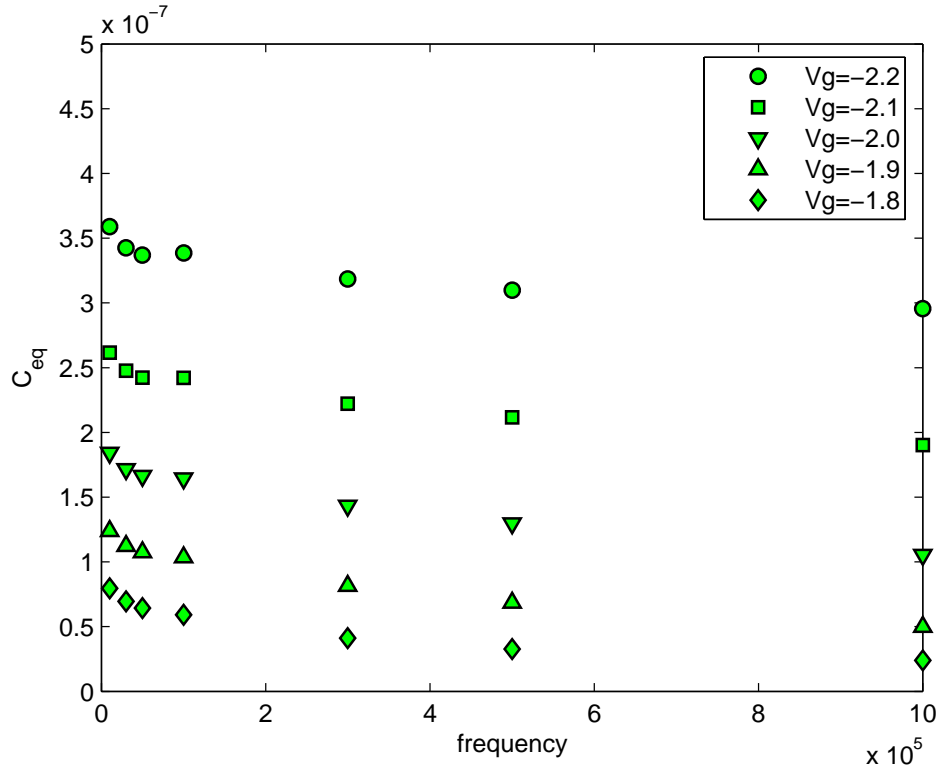
(a) Frequency response for $V_G = -2.2, \ldots, -1.8$.
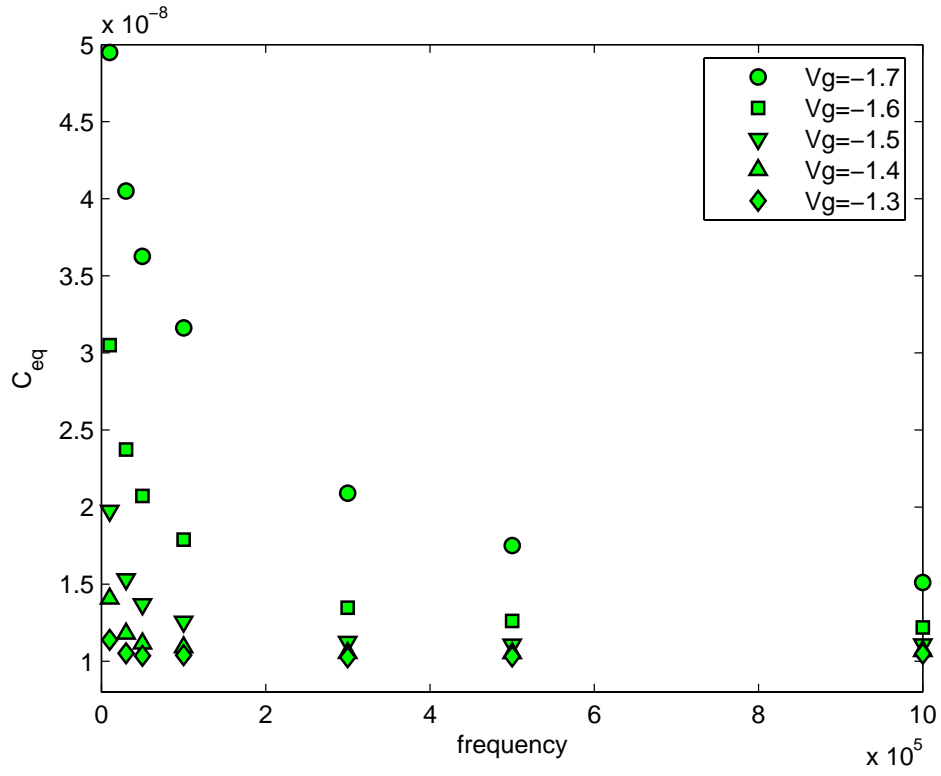
(b) Frequency response for $V_G = -1.7, \ldots, -1.3$.

Figure 7: Frequency response for TFTs.

in Figure 7, there are ten gate biases. Equation (7) indicates that there is a single pair of D_s and τ_s for all C_{eq} values, and for each set of C_{eq} values obtained under the same V_G, one pair of D_{it} and τ_{it} should be determined. There are 22 frequency response parameters. The objective value is also the sum of differences between the experimental data and the calculated results.

Without determining all the frequency response parameters simultaneously, we handle these parameters in separate groups. Because the values of C_{eq} are smallest when the gate bias is -1.3 or -1.4, higher accuracy is needed to determine the parameters for the two sets of experimental data. Therefore, in the first group, we determine D_s, τ_s, $D_{it}|_{V_G=-1.3}$, $\tau_{it}|_{V_G=-1.3}$, $D_{it}|_{V_G=-1.4}$, $\tau_{it}|_{V_G=-1.4}$. After obtaining D_s and τ_s, which are independent of V_G and f, we use the D_s and τ_s to determine D_{it} and τ_{it} for other gate biases. All rECGA parameters are identical to those in previous study cases, and the matching results are shown as the solid lines in Figure 8.

Figure 8 demonstrates that the matching results are remarkably satisfactory as the experimental data and the physical model pose a very difficult challenge for human to manually handle. Furthermore, based on the outcomes from the previous study cases, the pure random search has been decided inappropriate to handle the characteristic determination problem for solid state devices. As we can see in this work, the proposed framework of the real-coded ECGA, composed of ECGA and SoD, can be employed to tackle the characteristic determination problems of which the physical phenomena may be quite different.

4   Summary and Conclusions

In the paper, we proposed a new optimization framework by integrating the extended compact genetic algorithm (ECGA) and split-on-demand (SoD), an adaptive discretization method, to tackle the characteristic determination problem for solid state devices. Firstly, we briefly reviewed the key idea of ECGA and introduced the mechanism of SoD. Then, the real-coded ECGA (rECGA), which is an integration of ECGA and SoD, proposed in the present work was described in detail. We employed rECGA to handle three characteristic determination problems of which the physical phenomena and the mathematical models were different. The numerical results demonstrated that the proposed framework performed well on the study cases.

The characteristic determination problem is very important not only because the development of modern electronic computing equipment relies on solid state devices but also because more and more unknown physical phenomena are observed while the scale of the device gets smaller and smaller. In order to gain understandings of all these unknown phenomena, getting access to the parameters that cannot be directly measured or observed is of great assistance. With the help of methodologies in evolutionary computation, this paper offers a good approach for researchers and developers to deal with encountered characteristic determination problems effectively and efficiently.

Along this line of research, the immediate future work is to continue to apply the proposed framework on other problems emerging from the research on solid state devices. Moreover, in the process of extracting the desired parameters for the specific physical model, novel insights could be gained because computation of such an intensity is seldom utilized in this way to examine the existing physical models.

Acknowledgments
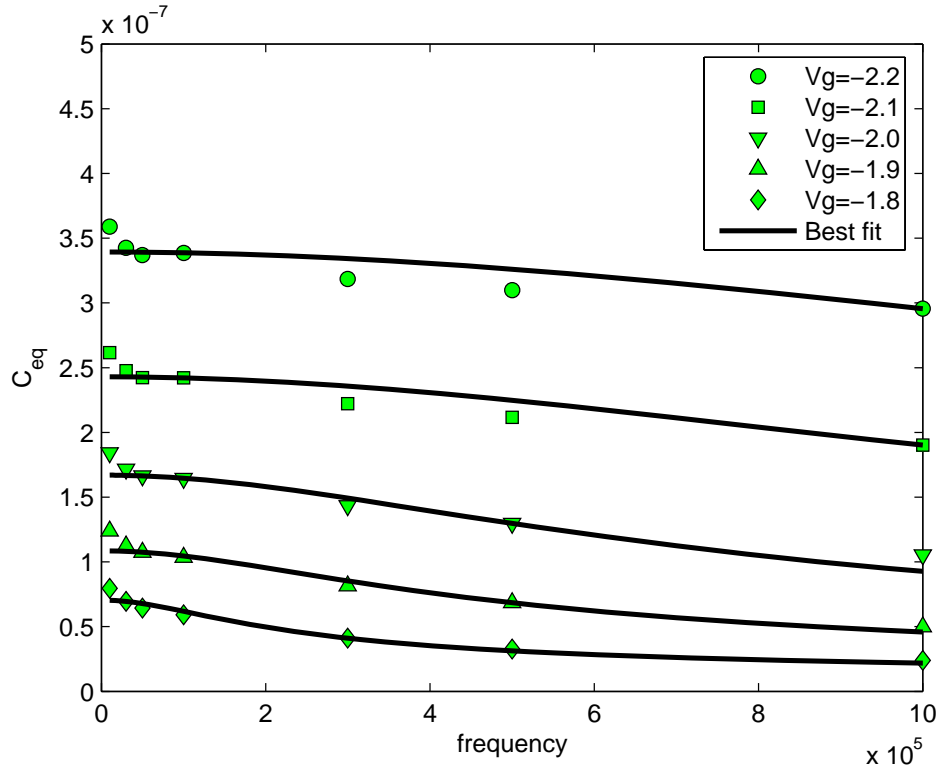
(a) Match results for $V_G = -2.2, \ldots, -1.8$.
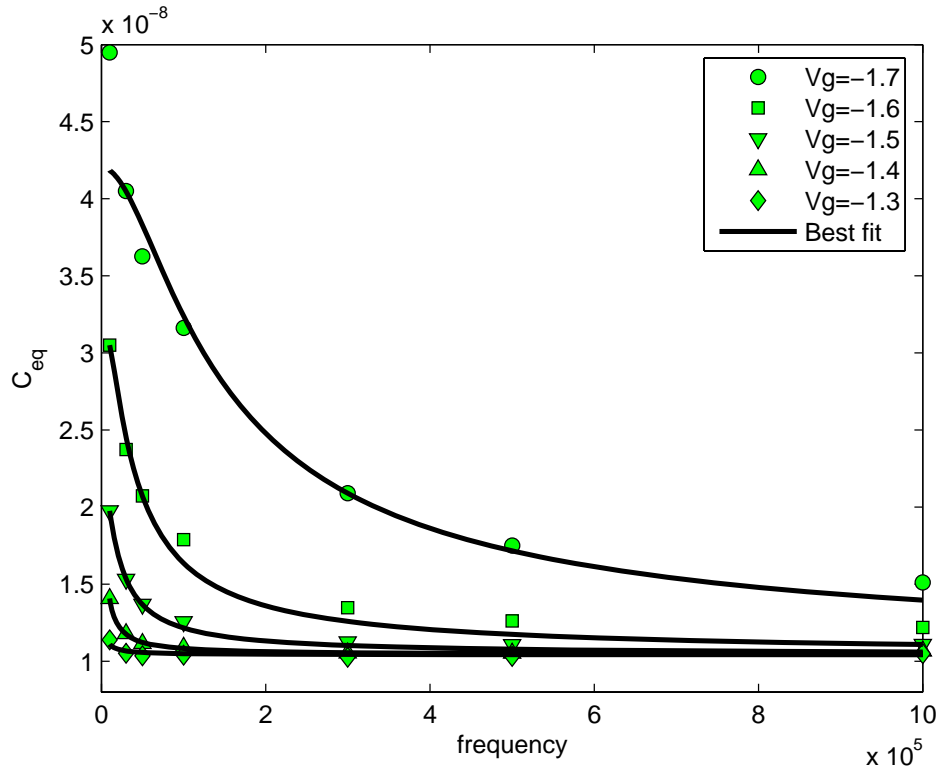
(b) Match results for $V_G = -1.7, \ldots, -1.3$.

Figure 8: Match results for the frequency response.

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