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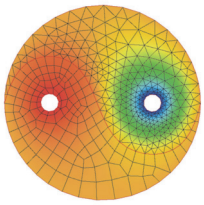

DEVICE SIMULATION AND MULTI-OBJECTIVE GENETIC ALGORITHM-BASED OPTIMIZATION OF GERMANIUM METAL-OXIDE-SEMICONDUCTOR STRUCTURE

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Abstract

Germanium (Ge) and high-κ dielectric materials draw many attentions due to their fascinating electrical characteristics comparing with silicon (Si) material. However, in physical and electrical simulation, the physical model may have deviation to reality case due to the process condition and manufacturing technology. To computationally study the device with Ge material, it is necessary to optimize the theoretical result with experimental data. This paper originally provides a new method to examine the static characteristic of Ge metal-oxide-semiconductor field effect transistors (MOSFETs) with aluminum oxide (Al_2O_3) by integrating device simulation, multi-objective evolutionary algorithm (MOEA), and unified optimization framework (UOF). To deal with the realistic problem, especially for the steep change of capacitance, we consider not only residual sum of squares (RSS) (i.e. the sum of squares of residuals) function but also physically crucial points in the optimization problem. Comparing to single-objective genetic algorithm (GA) with a weighted fitness, the preliminary result of this study shows the method has great improvement to optimize the suitable parameters which not only minimize the RSS of capacitance but also agree the key capacitance values from physical view.

Key words: germanium MOSFET, aluminum oxide, fitting, capacitance-voltage curve, residual sum of squares, device simulation, genetic algorithm, multi-objective evolutionary algorithm, unified optimization framework, non-dominating sorting genetic algorithm (NSGA-II)

1. INTRODUCTION

While the semiconductor industry is evolving, germanium (Ge) is a raised and crucial material due to its higher carrier mobility comparing with silicon (Si) material. High carrier mobility can provide superior on-state characteristic of metal-oxide-semiconductor field effect transistors (MOSFETs). Also, the process of Ge MOSFETs has high compatibility with process of silicon. Various high-κ insulating films are studied to boost the device's performance; among them, gate stack structures of $Al_2O_3/GeO_2/Ge$ could form low-defect high-κ oxide layers, where the GeO_2 layer is a suitable interfacial layer for realizing superior high-κ Ge interfaces (Zhang et al., 2012). Based on the experimentally measured data, we can estimate and achieve even better device design by using semiconductor device simulation with calibrated physical and structural parameters. However, the simulation result with the same experimental parameter input may differ from experimental results. The deviations depend on the process environment and the inaccuracy of physical model, thus the parameter values in simulator should vary in certain range. To accurately extract the crucial parameters, cost-effective ways used to optimize the results between simulation and targeted goal are necessary. Genetic algorithm (GA), a kind of evolutionary algorithm, is a globally-searching optimization method in a large population and its evolution

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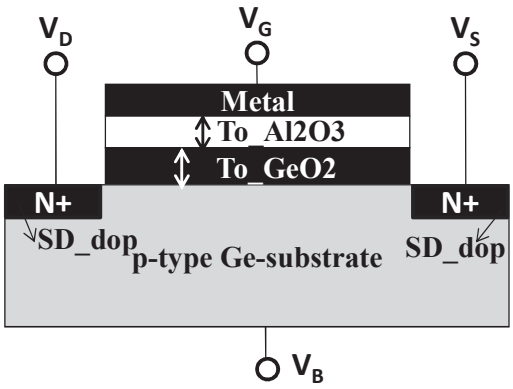
process is based on the mechanism of natural selection. Recent applications of GA in semiconductor devices (Li et al., 2011) and electronic circuits (Li et al., 2013) were reported and have shown remarkable achievements on design optimization. For real-world engineering optimization problems, there are many goals to be optimized at the same time. Therefore, we have to introduce a weighting factor for all concerned goals so that a single-objective function can be modeled empirically. However, to determine weighting factors for each goal may lead the original optimization problem to additional uncertainty. Intuitively, multi-objective problem (MOP) can find the optimal population for each objective on its own dimension without using any weighting factors (Bansal et al., 2013; Hariharan et al., 2014). Therefore, in contrast to diverse try-and-error methods, it will be an interesting study for us to optimize capacitance- voltage (C-V) curve of Ge MOS devices by using a device simulated based MOEA methods.

In this work, we implement a new method to automatically optimize the capacitance of Ge MOSFET with Al_2O_3/GeO_2 film by using a semiconductor-device-simulation-based MOEA method running in the unified optimization framework (UOF) (Li et al., 2008). The capacitance optimization problem with material-, structure- and process-related parameters can be formed as a multi-objective optimization problem. By minimizing each objective, the presented method can simultaneously optimize seven designing parameters successfully. This paper is organized as follows. In Section II, we introduce the studied Ge MOS. In Section III, we brief the problem modeling and the semiconductor-device-simulation-based MOEA method in the platform of UOF. Then, we report and discuss the optimization results obtained from GA and MOEA methods. Finally, we conclude this study and suggest future work.

2. THE EVOLUTIONARY METHODOLOGY

2.1. The Structure of Germanium Metal-Oxide-Semiconductor

The primary high-κ material is Al_2O_3 in the experiment sample. The GeO_2 layer is naturally generated from germanium substrate and is a satisfactory interfacial layer for realizing high quality interface between high-κ Ge substrate. Figure 1 shows the simulation structure to calculate the electrical characteristic of the Ge MOSFET. The device's channel length is fixed at 10 μm. The measured thickness of GeO_2 and Al_2O_3 layers are 3 nm and 5 nm, and the workfunction of metal gate is around 5 eV. We use two-dimensional (2D) device simulation with a small drain voltage and apply the gate voltage (V_G) ranging from -2 to 2 V. According to the physical observations, the entire gate capacitance – gate voltage (C_G-V_G) curve can be partitioned into three regions: the accumulation, the depletion, and the inversion regions. Some of the parameters are flexible to be varied including the dielectric constant and thickness of Al_2O_3 and GeO_2, the parameter to adjust doping profile in germanium substrate, the source/drain doping level, and the workfunction of metal gate induced by nanosized grain orientation which may vary due to different treatments of fabrication process.



Parameters to be optimized of the studied Ge MOS Structure

- Thickness of GeO_2 layer: ***To_GeO2*** (nm)
- Thickness of Al_2O_3 layer: ***To_Al2O3*** (nm)
- The ratio parameter of Gaussian doping : ***ratio_g***
- Doping concentration of the *source/drain doping*: **SD_dop** (cm^{-3})
- The dielectric constant of GeO_2: ***eps_GeO2*** ($CV^{-1}m^{-1}$)
- The dielectric constant of Al_2O_3 : ***eps_Al2O3*** ($CV^{-1}m^{-1}$)
- Workfunction of metal gate: ***WK_Metal*** (eV)

Fig. 1. *A 2D plot of the studied Ge MOS structure with the high-κ oxide layers. There are seven parameters to be optimized.*

With the purpose of exploring the physically transport operation in Ge MOSFET, three governing equations which include Poisson equation and current-continuity equations for electron and hole transportation in semiconductor are solved self-consistently (Li, et al., 2002). The equations indicate that the number of carriers is conserved and the electrostatic potential due to the carrier charges obeys Poisson's equation.

2.2. The Integrated Device Simulation, MOEA, and UOF Methodology

Based on our earlier developed unified optimization framework (UOF), we utilize integrated MOEA and numerical semiconductor device simulator to approach the experimental data of Ge MOSFET. This framework provides flexible interfaces to deal with different optimization method and numerical simulation solver, enabling these two different research fields to be bridged. The components of the UOF consist of several classes for different purpose; two primary classes are adapted for diverse problem and solver components, as shown in figure 2. The corresponding numerical simulation tool is defined in the problem class and the optimization algorithm is in the solver components. These two parts can be adjusted independently allowing high-level code to be reused, and rapidly adapted to other problems and algorithms.

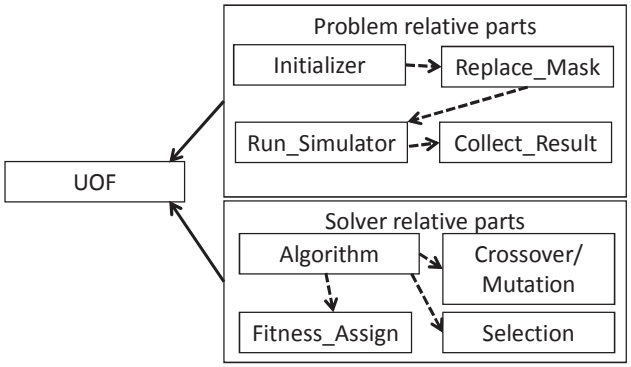


Fig. 2. *The class components of unified optimization framework (UOF).*

Figure 3 shows the built-in class specializations of the most important two classes in current UOF. As shown in figure 3a, NPProblem, FunctionProblem, and ExtSimProblem are directly inherited from UOFProblem. The UOFProblem class has general interfaces for the user to define any problems. NPProblem provides convenient interfaces for defining NP-hard problems such as TSP and the single/parallel machine scheduling problem. Moreover, optimization problems of linear and non-linear continuous functions can be defined by FunctionProblem class. The population-based solver includes several heuristic methods such as GABaseSolver for genetic algorithm (GA), PSOSolver for particle swarm optimization (PSO) (Kennedy & Eberhart, 1995), ACOSolver for ant colony optimization (ACO) (Dorigo & Gambardella, 1997) and multi-objective evolutionary method (MOEA) (Deb et al., 2002).

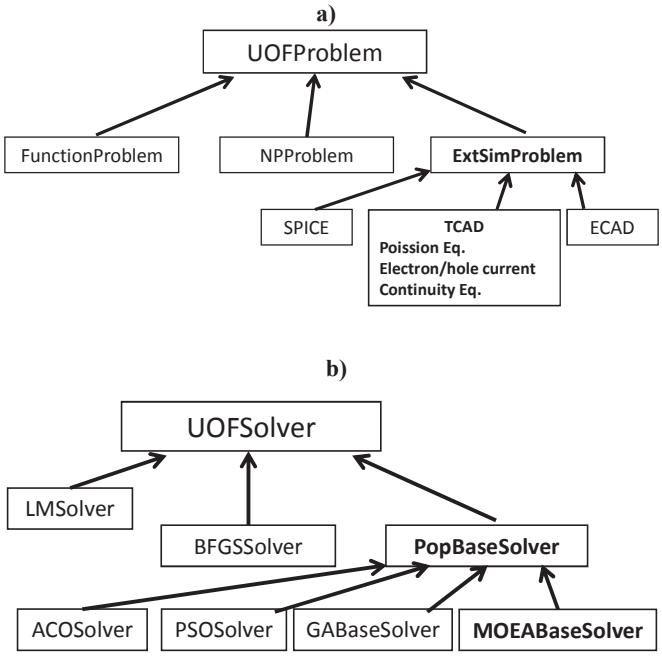


Fig. 3. *The concept of class hierarchy of the UOFProblem (a) and UOFSolver (b). The solid lines indicate inheritance. TCAD and MOEABaseSolver are used in this work.*

Because the UOF is based on C++ language and consists of several classes, it has high coding flexibility. The class to call simulator and the class to call optimization algorithm are separated, thus we can achieve different simulators and algorithm to solve various problems. The program "main" governs the process step of optimization flow, as listed below.

```
void main
{
1. Set max iteration count, min error, population size, cross rate, mutation rate
2. Readfiles( fileList ) // file list contains
   // the name of intermediate file, input
   // and output file of simulator
3. ReadSetting( configure file) // configure
   // file contain cross/mutation rate,
   // command for simulator, and the key
   // word in output files.
4. Problem GeMOSCV()
5. Algorithm NSGAII()
6. NSGAII→iteration
}
```

To achieve the device characteristic of the individuals, as listed below, we replace the values in simulator file by the values of population. For each population, the simulation parameter values are set and then the device characteristic is solved by simulation tool. While the simulation is finished, the value of characteristic are obtained by simulator and recorded the results in its own output files. The sub

function defined in the problem class can receive the values in certain output file. Then, it calls the function defined in algorithm to assign fitness of the individuals.

```
void Problem: Run_Simulator
{
1. Remove old results
2. Real values of individuals
3. Replace these values into intermediate
   file
4. Call TCAD and solve Poisson and elec-
   tron/hole current continuity equations
5. Collect Result
}
```

In this work, we implement the non-dominating sorting genetic algorithm (NSGA-II) in algorithm class. The computational complexity of NSGA-II is $O(MN^2)$, where M is objective number and N is the population size. In addition to technically sorting by several fronts, NSGA-II defines crowd distance to ensure that the Pareto front can keep a good diversity. The components of algorithm class are listed below.

```
Class Algorithm
{
void Selection, Crossover, Mutation
void Evaluation
bool Dominate
void CrowdDistance
}
```

In this work, we consider several objectives, including the six crucial values of the C-V curve. The C_{Lmax} is the capacitance value for the lowest measured gate voltage, the C_{slope} is the most negative slope for capacitance decrease while the gate voltage increase, the V_{Cslope} is the gate voltage where the capacitance is C_{slope}, the C_{min} is the minimum capacitance value of entire curve and the V_{Cmin} is its corresponding gate voltage, and the C_{Rmax} is the capacitance value for the highest measured gate voltage. The deviations of these values between the simulation result and given specs are considered as objectives directly. Our ultimate goal is achieving the goal capacitance perfectly by adjusting the most crucial material/structure parameters, so we define RSS as the sum of square to summarize the capacitance-value deviation between the simulation result and the given specification. The seven objective functions are all minimization problem since the results can fit the target well if all deviations are zero. The objectives are given by:

$$Objective\_1 \equiv C_{L\max t} - C_{L\max,spec} \quad (1)$$

$$Objective\_6 \equiv V_{C\min} - V_{C\min,spec} \quad (2)$$

and

$$Objective\_7 \equiv \min \sum_{v=-2}^{2} r_v(C_v)^2 \quad (3)$$

where $r_v(C_v) = C_v - C_{v,spec}$. In this study, two strategies are applied to include these objectives; one is combining these objectives by weighting coefficients while another is directly using multi-objective evolutionary algorithm with all objectives at the same time.

3. RESULTS AND DISCUSSION

The optimization problem in this work is nonlinear and is not exactly formulated, that's the reason we use the simulation-based technique. If we use GA and consider only RSS, it's hard to promise an acceptable deviation between simulation result and specification. To lead the evolution process to match the spec curve eventually, we consider physical key parts of C-V curve as well as RSS and use empirical weighted sum to model the problem into a single-objective fitting problem. The achieved results from GA and MOEA are shown in figure 4, we select the result with the minimum RSS in the population of the last generation. This diagram shows that adding those key consideration points to adjust the fitness can achieve desirable approach with small RSS by both two methods. Because these objectives have mutual interference and relate to different set of parameters, the fitting curve has inevitable difference to the specified curve. Once we have some objectives optimized by this way, the results are based on this set of weighting parameters. If we try to optimize other objectives, it is a difficult process to obtain another set of weighting coefficients. Although the RSS can be minimized by more evolutionary generations, the shape of C-V curve cannot be satisfied from device engineering's view point for some gate bias region. Although the objective can be scaled and emphasized, the results still cannot highlight those important points simultaneously. The MOEA which use all objectives directly can achieve even better optimized result comparing with GA

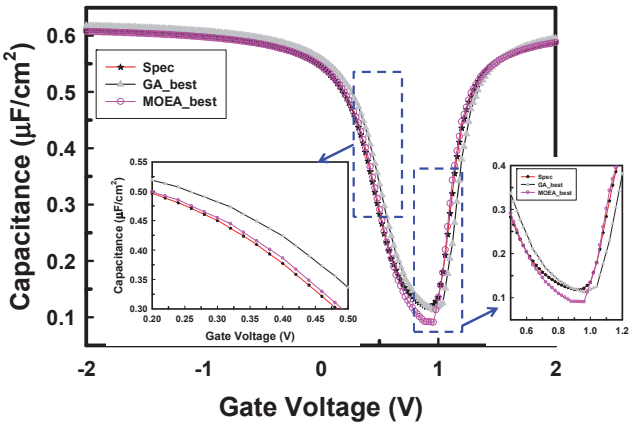


Fig. 4. The optimized results by using the weighted objective sum and GA.

proved. We can find strong coupling between the capacitance and designing parameters around C_{min} region. As shown in figure 4, the comparison of results between GA and MOEA indicates the semiconductor-device-simulation-based MOEA method is computationally effective to handle the complex curve shape with suitable objectives. The reason is that the MOEA method can approach several characteristic with respect to each objective function; consequently, the optimization process governed not only by RSS but also the physical objectives.

Figures 5a-d show the optimized $|C_{min}-C_{min,spec}|$ versus $|C_{slope}-C_{slope,spec}|$ from the MOEA. We observe two important objectives, $|C_{min}-C_{min,spec}|$ and

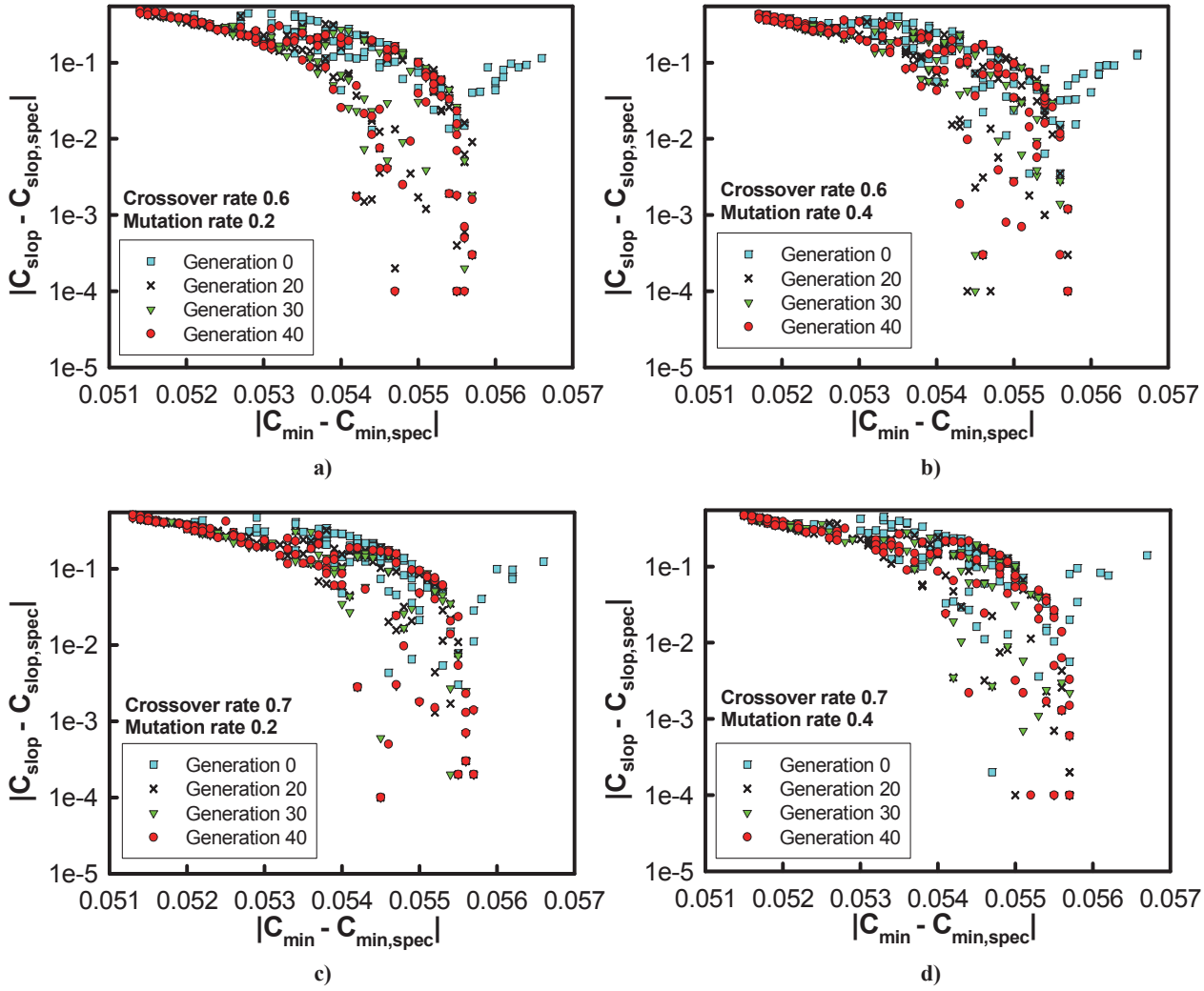


Fig. 5. The optimized result of MOEA with different evolution settings.

method. The optimized curve fits the specified curve well everywhere. It is worth mentioning that the generation of MOEA method still keeps great diversity, meaning that the population will be continuously improved for more generations. In particular, results of the neighborhood of C_{min} which is the most physically complex point in the curve can be im-

$|C_{slope}-C_{slope,spec}|$ which determine the behavior near the point C_{min} and are mutual interference. These four plots show the results of MOEA method under different crossover rate and mutation rate. The population moves toward smaller objective value with more iteration. The achieved Pareto fronts under four optimization settings are very similar. If we

increase mutation rate, as shown in figures 5a and b, individuals may move away from the Pareto front to find other potential optimizers. On the other hand, high crossover rate makes the individuals evolve near the Pareto front and achieve smooth Pareto front surface, as shown in figures 5a and c.

4. CONCLUSIONS

In this study, based upon a unified optimization framework, an alternative way to optimize high-κ Ge MOSFET has been reported by using a semiconductor-device-simulation-based MOEA method. The MOSFET's C_G-V_G curve optimization problem has been modeled as a MOP with simultaneously considering capacitance's physical constraints. Different from conventional try-and-error tuning method in device engineering, the main findings of this study indicate that the semiconductor-device-simulation-based MOEA method not only enables us to approach the capacitance in accumulation, depletion, and inversion regions of Ge MOSFET, but also achieves better results than the GA's results. Notably, the MOEA method can effectively capture the complicated curve's behavior compared with the GA method. The GA with a single-objective function strongly depends on empirically estimated weighted sum of multi- objectives which is difficult for real-world applications. We are currently using this method to optimize and design new experiments.

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SYMULACJA I WIELOKRYTERIALNA OPTYMALIZACJA ALGORYTMEM GENETYCZNYM PÓŁPRZEWODNIKOWYCH STRUKTUR TLENKU GERMANU

Streszczenie

German (Ge) i materiały o wysokiej stałej dielektrycznej są interesujące ze względu na swoje niezwykle ciekawe charakterystyki elektryczne w porównaniu do krzemu (Si). Jednakże w symulacjach fizycznych i elektrycznych, model fizyczny może odbiegać od przypadku rzeczywistego ze względu na warunki procesu i technologię produkcji. Badania z wykorzystaniem metod obliczeniowych dla urządzeń wykonanych z germanu wymagają optymalizacji wyników teoretycznych z danymi doświadczalnymi. W pracy zaproponowano metodę badania statycznych charakterystyk tranzystorów polowych z tlenku germanu – półprzewodnika (MOSFETs) z tlenkiem aluminium (Al_2O_3), z wykorzystaniem zintegrowanego systemu składającego się z urządzenia do symulacji charakterystyk elektrycznych półprzewodników, wielokryterialnego algorytmu ewolucyjnego (MOEA) oraz zunifikowanej platformy do optymalizacji (UOF). Dla rozwiązania rzeczywistego problemu, zwłaszcza przy gwałtownej zmianie pojemności, w zadaniu optymalizacji rozważano nie tylko sumę kwadratów reszt (RSS), ale również kluczowe, z punktu widzenia fizyki, aspekty. W porównaniu z jednokryterialnym algorytmem genetycznym (GA) z ważoną funkcją dopasowania, wyniki przeprowadzonych badań pokazały, że opracowana metoda, która minimalizuje nie tylko błąd RSS dla pojemności, ale także bierze pod uwagę kluczowe wartości pojemności z fizycznych obserwacji, znacznie poprawiła zadanie optymalizacji wybranych parametrów zagadnienia.

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