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Estimation of Physical Properties of Si by Laser Heterodyne Photothermal Displacement Method and Machine Learning

Shota Urano†, Tomoki Harada*, Tetsuo Ikari, and Atsuhiko Fukuyama
(Faculty of Engineering, Univ. of Miyazaki)

1. Introduction

The Demand for data storage and information processing technologies is increasing toward the realization of Society 5.0. As a result, semiconductor devices are required to have higher speed and functionality, and semiconductors are becoming increasingly miniaturized and highly integrated. Thus, generated heat in semiconductor devices is increased. On the other hand, heat generation due to nonradiative recombination is also considered as one of the factors. This is a problem because it leads to performance degradation and low lifespan of semiconductor devices. In order to control the heat generation, it is necessary to properly evaluate the physical properties related to nonradiative recombination of the semiconductor material. We have been evaluating semiconductors by using piezoelectric photothermal (PPT) method[1)] to detect thermal expansion and thermal waves of a sample due to nonradiative recombination of photoexcited carriers with high sensitivity. However, the PPT method is difficult to evaluate quantitatively because the signal intensity varies depending on the mounting conditions of the sample and the piezoelectric element. Therefore, we developed the laser heterodyne photothermal displacement (LH-PD) method[2)], which is a nondestructive and noncontact method to measure the thermal expansion displacement of a sample surface due to the heat generation with the nonradiative recombination of photoexcited carriers by a heterodyne interferometer. Furthermore, time-resolved measurement of the displacement is possible, and the time variation of the displacement includes information on physical properties such as optical absorption coefficient, thermal diffusivity, carrier mobility, and carrier lifetime. Therefore, each physical property value can be estimated by fitting analysis of the time variation of displacement. Theoretical calculations were performed to reproduce and fit the time variation of displacement using COMSOL Multiphysics®[3)], which is simulation software. However, due to the large number of parameters involved, the fitting process requires a great deal of time and effort. Therefore, the purpose of this study is to develop a rapid estimation for the physical property from the time variation of the displacements using machine learning.

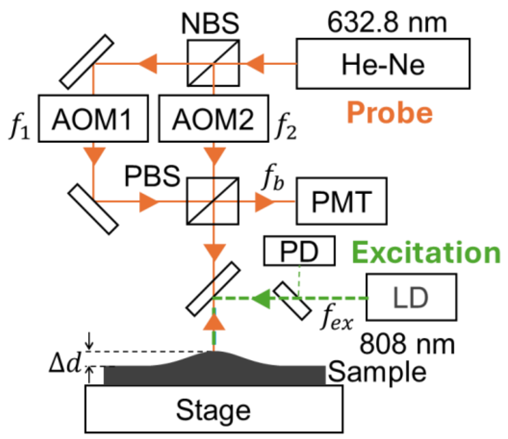

Fig.1 Schematic diagram of LH-PD equipment.

2. Experimental and Theoretical calculation

Figure 1 shows a schematic diagram of the LH-PD method. A semiconductor laser diode (LD) with a wavelength of 808 nm was used as the excitation light, and a He-Ne laser with a wavelength of 632.8 nm was used as the detection light. The detection light was split into two optical paths by a nonpolarizing beam splitter (NBS). Their frequency was modulated by an acoustic optics modulator (AOM) with frequencies f_1 and f_2, respectively. The f_1 was used as the reference light, and after passing through the polarizing beam splitter (PBS), it entered the photomultiplier tube (PMT). The f_2 is used as the probe light, and after passing through the PBS, it is reflected on the sample surface. It then merges with the reference light to form a beat signal ($f_b=|f_1-f_2|$). The beat signal is converted into an electrical signal by PMT and detected. At the same time, 5% of the excitation light is extracted by a beam sampler and detected by a Si photodiode (PD) as a reference signal. In the LH-PD method, the irradiation position of the excitation and the detection light can be controlled. Hereafter, the distance between the two irradiation positions is referred to as the irradiation distance.

Theoretical calculations taken into account the generation carriers, diffusion, and nonradiative recombination of photoexcited carriers, heat

E-mail: †hk20003@student.miyazaki-u.ac.jp,
*tomoki.harada.q5@cc.miyazaki-u.ac.jp

diffusion, and thermal expansion. In other words, the carrier continuity equation, the thermal diffusion equation, and the elastic equation were solved to reproduce the time variation of the displacement. Since these phenomena are axisymmetric with the excitation light, a cylindrical coordinate system was used to calculate.

3. Machine Learning Methods

The input data for machine learning were generated by substituting random values of four physical properties (thermal diffusivity, carrier mobility, carrier lifetime, and surface recombination velocity) in *n*-type Si substrate into theoretical calculations under two conditions of 0 and 50 µm irradiation distance. 2000 data sets ware prepared with aforementioned four physical properties and the time variation of the displacement. They are divided into training data (60%), validation data (20%), and test data (20%). A fully connected feedforward neural network model was constructed and trained using the Keras[4] and TensorFlow[5] library in Python. The input data of neural network model were the time variation of displacement and the surface recombination velocity, and outputs were one of the following: thermal diffusivity, carrier mobility, or carrier lifetime. The two physical property values not used for the output were entered in the middle of the model. A rectified liner unit[6] was applied to the activation function, and loss was measured by mean squared error of the outputs.

4. Result

Figure 2 shows the relationship between the set values and predicted values of (a) thermal diffusivity, (b) carrier mobility, and (c) carrier lifetime for the test data. The diagonal lines in the figure indicate that the set values and predicted values are equal, and the more the plotted data is on the diagonal line, the higher the estimation accuracy. The root mean square error (RMSE) of the thermal diffusivity is 0.022 (m^2/K) and the coefficient of determination (R^2) is 0.998. The RMSE of carrier mobility is 0.125 (cm^2/V・s) and R^2 is 0.978. The RMSE of carrier lifetime mobility is 0.127 and R^2 is 0.992. The obtained estimation accuracy was sufficient for practical evaluation, and the learned model enabled property estimation in a few seconds.

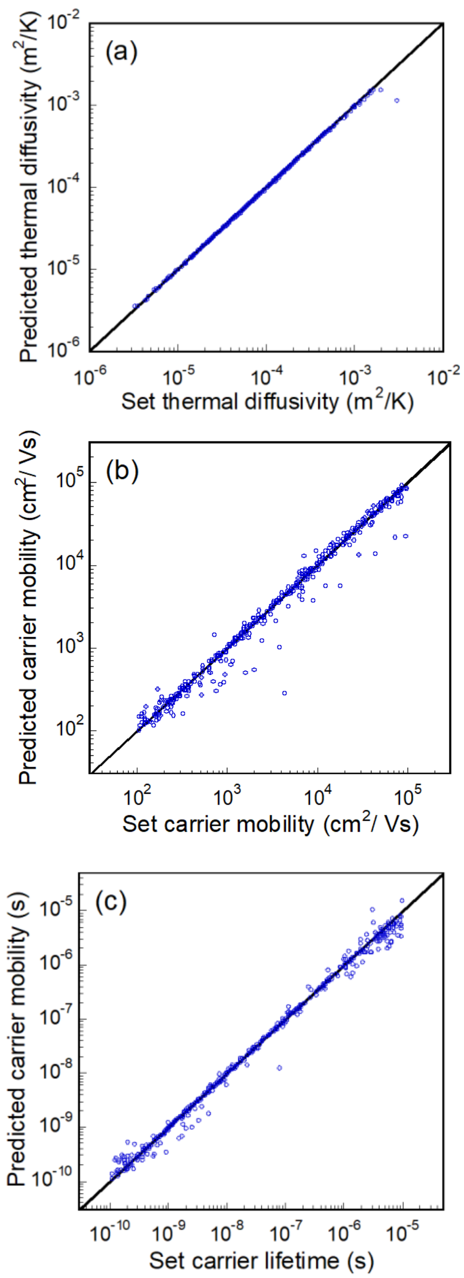

Fig.2 Prediction results of each property value.

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