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Theoretical study on the photothermal signal of the multilayer structure and application to the Si-nanopillar/SiGe composite films

多層構造体の光熱変換信号理論の検討と Si ナノピラー/SiGe 複合膜への適用

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1. Introduction

Piezoelectric phptothermal (PPT) technique can detects the thermal and elastic waves generated by the nonradiative recombination of photoexcited carriers in the semiconductor. In our previous works, we discussed the decreasing the thermal conductivity (κ) in highly-periodic Si-nanopillars (NP) embeded in SiGe matrix (Si-NP/SiGe) fabricated by using bio-template and neutral beam etching[2)]. We had concluded that κ of Si-NP/SiGe composite film was significantly smaller than that of bulk Si[3)]. However, the heat propagation whitin the $LiNbO_3$ transducer and surrounded air had not been considered. If the heat escaped to the surrounded air, the past estimated value was not appropriate. Therefore, we developed our analysis by taking into account the heat propergating whitin the transducer and escaping to the outside.

2. Experimental method

The procedures of the sample preparation have already been reported[3, 4)]. The Si-NPs with diameter of 10 nm embedded in $Si_{0.7}Ge_{0.3}$ were fabricated on Si-on-insulator substrate. The density of Si-NPs was 1.6×10^{11} cm^{-2}. For PPT measurements, the probing light was illuminated on the Si substrate side and generated thermal and elastic waves caused by the non-radiative recombination were detected by $LiNbO_3$ transducer that directly attached to the Si-NP/SiGe composite film side. Since the propagation of thermal and elastic waves were hindered by Si-NP/SiGe film before reaching the detector, the PPT signal intensity decreased. We have carried out the PPT measurements at room temperature by changing the chopping frequency of the probing light (f) from 40 to 3500 Hz. The wavelength of the probing light was fixed at 1120, 1090, 1060, and 1030 nm. The theoretical analysis based on the one-dimensional thermal propagation in multilayer structure was carried out.

Figure 1 shows a schematic model for present theoretical calculations. The temperature within the i-th layer ($T_i(x_i)$) is given by solving the one-dimensional heat diffusion equation[5)],

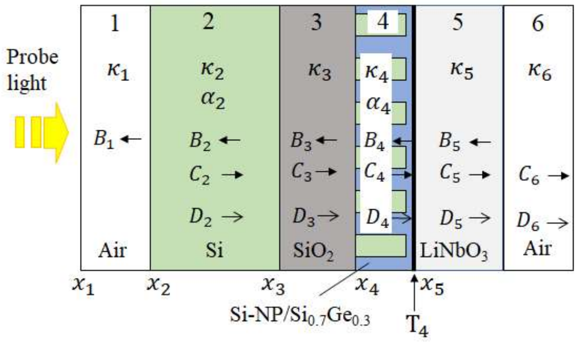

Fig. 1 The schematic figure of theoretical model

$$T_i(x_i) = \exp(j\omega t)[B_i exp\{\mu_i(x-x_i)\} + C_i exp\{-\mu_i(x-x_i)\} + D_i exp\{-\alpha_i(x-x_i)\}], \quad (1)$$

where j is the imaginary unit, ω is the angular frequency, t is time. B_i and C_i indicate the amplitude of thermal waves in i^{th} layer propagation toward i - 1th layer and i + 1th layer, respectively. D_i is the temperature rise due to the light absorption in the i^{th} layer. μ_i and α_i are the thermal diffusion coefficient and the optical absorption coefficient in the i^{th} layer, respectively. By substituting eq. (1) into heat diffusion equation, following relations are obtained,

$$\mu_i = (1+j)/\lambda_i \quad (2)$$

$$\lambda_i = (2\kappa_i/\omega\rho_i c_i)^{1/2} \quad (3)$$

$$D_i = -\alpha_i I_i / \left(\kappa_i(\alpha_i^2 - \mu_i^2)\right), \quad (4)$$

where λ_i is the thermal diffusion length. κ_i, ρ_i and c_i are the thermal conductivity, density and specific heat, respectively.

We supposed that the PPT signal intensity is proportional to the temperature at the interface between Si-NP/SiGe composite film and $LiNbO_3$. Therefore, we calculated $T_4(x_5)$ in the model

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shown in Fig.1. The 6th air layer was considered by taking into account the heat propergating whitin the transducer and escaping to the outside. The physical parameter of Air, Si, SiO_2 and $LiNbO_3$ were taken from literature[6, 7)]. In addition, we assumed that α of Air, SiO_2 and $LiNbO_3$ were negligibly small. As a result, the fitting parameters were only κ_4 and α_4 of Si-NP/SiGe composite film.

3. Result and discussion

Figure 2 shows the f -dependence of the experimental and theoretically calculated PPT signal intensities for two conditions at wavelength of 1090 nm. Experimental data were already reported in the previous papers[3,4)]. At low f region, the PPT signal intensity was decreased as f increased. This is because λ_i is proportional to a reciprocal square root of f. However, at high f region, a distinct dip was observed around 800 Hz. The calculated PPT signal intensities as a function of f using the present model are also shown. As shown in this figure, calculated PPT signal intensities well reproduced the experimental results. For considering the effect of 6th layer, we also calculated the PPT signal using the model without the 6th layer. No difference was observed for the calculated curves. This implies that the heat propergation whitin the transducer and escaping of heat outside are negligibly small.

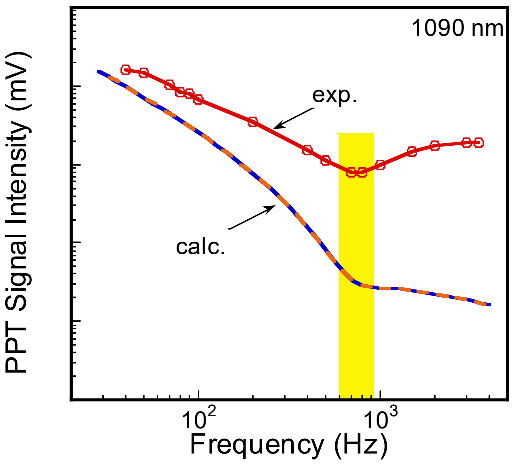

Fig. 2 $\boldsymbol{f}$-dependency of experimental and theoretically calculated PPT signal intensities

For detailed discussion, we separately calculated B_4 and C_5 at the interface x_5 (between Si-NP/SiGe composite film and $LiNbO_3$). In this case, B_5 is the amplitude of thermal wave in $LiNbO_3$ towards Si-NP/SiGe and C_4 is that in Si-NP/SiGe towards $LiNbO_3$. They were estimated to be around 50 and 2.5×10^{-3}, respectively, for both models with and without the 6th air layer. These results implied that almost thermal waves in Si-NP/SiGe composite film were reflected at the interface x_5. This may be caused by the low value of thermal conductivity of $LiNbO_3$ of κ_5 = 0.0353 (W/cmK)[6)]. As a result, thermal wave in $LiNbO_3$ was extremely small and did not affected by the presence of the 6th air layer. However, for high-sensitivity detection of thermal wave in Si-NP/SiGe composite film, a transducer with relatively high value of κ_5 is necessary.

4. Conclusion

We have carried out the PPT measurements of Si-NP sample and theoretical analysis for multilayer structure based on one-dimensional heat diffusion equation. Calculated results well reproduced the experimental f -dependence of the PPT signal intensities. We also investigated the effect of heat propagation between the $LiNbO_3$ and rear-side air layer as well as at the interface of Si-NP/SiGe composite film and $LiNbO_3$. In conclusion, since the thermal conductivity of $LiNbO_3$ was small, an effect of heat propagation within the $LiNbO_3$ and escaping to the rear-side air is found to be negligibly small.

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