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Note

Application of Combined Experimental and Numerical Techniques in Determining the Temperature Dependence of Reflectivity of Semiconductors

R. Černý,[1,2] V. Cháb,[3] and P. Přikryl[4]

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Combined experimental and numerical techniques for determining the temperature dependence of reflectivity of basic semiconductors are analyzed. The method for determination of the reflectivity dependence of liquid semiconductors under pulsed laser irradiation on temperature developed earlier by the authors is modified for the case of solid semiconductors. The results obtained by the time-resolved reflectivity measurement technique together with the known temperature dependencies of the refraction index and the extinction coefficient for the cw probe laser and the room-temperature data for the reflectivity at the frequency of the primary pulsed laser beam are the input parameters of this method. The method itself consists in matching the experimental and computed values of the maximum reflectivity of cw probe laser in dependence on the energy density of the laser pulse and a least-squares fitting procedure. The method is verified on experimental data for the XeCl excimer laser irradiation of Si(100), giving $R_s = 0.590 \pm 0.005 + (4.5 \pm 0.5) \times 10^{-5}(T - 293)$ for the reflectivity of crystalline silicon, which is in good agreement with experimental measurements done by other investigators. In addition, numerical test and error analyses of both the method presented here and the previous method proposed for liquid semiconductors are described and the accuracy and error limits of both methods are discussed.

KEY WORDS: pulsed laser; reflectivity; semiconductors; time-resolved reflectivity technique.

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[1] Faculty of Civil Engineering, Czech Technical University, Thákurova 7, 16629 Prague 6, Czech Republic.

[2] To whom correspondence should be addressed.

[3] Institute of Physics, Academy of Sciences of the Czech Republic, Na Slovance 2, 18040 Prague 8, Czech Republic.

[4] Mathematical Institute, Academy of Sciences of the Czech Republic, Žitná 25, 11567 Prague 1, Czech Republic.

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1. INTRODUCTION

Optical properties of indirect-gap semiconductors such as silicon change markedly with temperature and wavelength [1]. In measuring the dependence of the refraction index and extinction coefficient on the wavelength, scanning ellipsometry techniques are commonly employed [2, 3]. Using analogous methods for determining the dependence of optical properties on temperature is also possible [3–5]. To obtain detailed information about this dependence is, however, a very time-consuming task.

Therefore, alternative treatments have been studied during the past 10 years (see, e.g., Refs, 6–8). Recently, it was shown [9] that using the time-resolved reflectivity (TRR) technique at pulsed laser irradiation of semiconductor thin films in combination with the mathematical model of this experimental situation accounting for an optically nonhomogeneous medium [10] might be a very promising technique to determine an approximate reflectivity-vs.-temperature relation of liquid semiconductors at high temperatures.

In this paper, we modify the method given in Ref. 9 for the case of solid materials and develop a procedure for determining the dependence of the reflectivity of solid semiconductors on temperature based on TRR measurements and room-temperature reflectivity data for the primary laser. Moreover, we present numerical tests and an error analysis of this method compared with the method for determining the reflectivity of liquid semiconductors [9] and discuss the errors associated with each method.

2. ALGORITHM FOR DETERMINING THE REFLECTIVITY OF SOLID SEMICONDUCTORS

Similary to the method for determining the reflectivity of liquid semiconductors described in Ref. 9, we assume the following experimental situation: a semiconductor sample is irradiated by a pulsed laser, and a cw probe laser is focused onto the irradiated spot on the sample surface. Time-resolved reflectivity of the cw laser is measured during the pulse of the primary laser. We assume that the reflectivity of the primary laser is known at room temperature but not at elevated temperatures, while the reflectivity of the cw laser is known over the temperature range considered.

Using the thermal model of laser processing of semiconductors of Černý et al. [10], we are able to generate numerical equivalents of the TRR curves obtained experimentally and to determine their maxima, $R^{\mathrm{P}}_{\mathrm{max,\,c}}$. Calculating these maxima for various energy densities E of the primary laser, we obtain $R^{\mathrm{P}}_{\mathrm{max,\,c}}$ as a function of E. As a result of TRR measurements, we can obtain the same function determined experimentally,

$R^{\mathrm{P}}_{\mathrm{max}} = R^{\mathrm{P}}_{\mathrm{max}}(E)$. This fact can be employed in matching the experimental and simulated data for $R^{\mathrm{P}}_{\mathrm{max}}$.

The algorithm for determination of the reflectivity of solid semiconductors, R_{s}, is as follows.

(1) Compute the value of $R_{\mathrm{s0}} = R_{\mathrm{s}}(T_{\mathrm{R}})$, where T_{R} is the room temperature, $T_{\mathrm{R}} = 293$ K, from the known values of the refraction index n_{s} and the extinction coefficient k_{s}.

(2) Choose the type of $R_{\mathrm{s}}(T)$ function, e.g., $R_{\mathrm{s}}(\bar{T}) = R_{\mathrm{s0}} + A(\bar{T} - T_{\mathrm{R}})$, where the characteristic temperature $\bar{T}$ is defined by

$$\bar{T}(t) = \frac{(\int_0^{Z_0} T(x, t) \exp[-\int_0^x \alpha(\eta)\, d\eta]\, dx)}{(\int_0^{Z_0} \exp[-\int_0^x \alpha(\eta)\, d\eta]\, dx)}$$

Here Z_0 is the characteristic domain width obeying the condition $T(x, t) = T_0$ at $x > Z_0$.

(3) Choose a set of proper values $A = A_i$, $i = 1, 2, \ldots, n$.

(4) Compute $R^{\mathrm{P}}_{\mathrm{max,\,c},\,i}(E_i)$ for all experimentally given $E_i < E_{\mathrm{m}}$, where E_{m} is the melting threshold, and all A_i.

(5) Compute the error limits of $R^{\mathrm{P}}_{\mathrm{max,\,c}}(E)$ due to the errors in the input parameters of the model.

(6) For all values of A, compute the quantity $LS = (1/m^2) \sum_{j=1}^{m} [R^{\mathrm{P}}_{\mathrm{max,\,c},j}(E_j) - R^{\mathrm{P}}_{\mathrm{max},j}(E_j)]^2$, where m is the number of experimentally determined values of $R^{\mathrm{P}}_{\mathrm{max}}$ for $E < E_m$.

(7) Find $LS_{\mathrm{min}} = \min(LS(A_i), i = 1, 2, \ldots, n)$, and put $A = A_{\mathrm{min}}$, where A_{min} is the value of A_i corresponding to the LS_{min}.

(8) Discuss the error bars of both $R^{\mathrm{P}}_{\mathrm{max,\,c}}(E)$ computed with $A = A_{\mathrm{min}}$ and $R^{\mathrm{P}}_{\mathrm{max}}(E)$. If there are overlapping parts of these two error bars over the whole range of energy densities considered, accept A as the solution of the fitting procedure.

(9) Compute the correlation coefficient r as a test of the goodness of fit,

$$r = \frac{m \sum_{j=1}^{m} R^{\mathrm{P}}_{\mathrm{max},j} R^{\mathrm{P}}_{\mathrm{max,c},j} - \sum_{j=1}^{m} R^{\mathrm{P}}_{\mathrm{max},j} \sum_{j=1}^{m} R^{\mathrm{P}}_{\mathrm{max,c},j}}{\sqrt{[m \sum_{j=1}^{m} {R^{\mathrm{P}}_{\mathrm{max},j}}^2 - (\sum_{j=1}^{m} R^{\mathrm{P}}_{\mathrm{max},j})^2][m \sum_{j=1}^{m} {R^{\mathrm{P}}_{\mathrm{max,c},j}}^2 - (\sum_{j=1}^{m} R^{\mathrm{P}}_{\mathrm{max,c},j})^2]}} \qquad (1)$$

where $R^{\mathrm{P}}_{\mathrm{max},j}$ are the experimental values of $R^{\mathrm{P}}_{\mathrm{max}}$, $R^{\mathrm{P}}_{\mathrm{max,\,c},j}$ are the computed values of $R^{\mathrm{P}}_{\mathrm{max}}$, and m is the number of the experimental measurements.

3. RESULTS AND DISCUSSION

The TRR measurements were performed using the experimental setup described in Ref. 11, with samples of Czochralski-grown (100) orientation monocrystalline silicon (c-Si), primary XeCl excimer laser (308 nm, 27 ns FWHM), and HeNe probe laser (633 nm). Experimental TRR curves were determined in the range of energy densities of $E \in [0.4\ \mathrm{J\cdot cm^{-2}}, 0.7\ \mathrm{J\cdot cm^{-2}}]$. The reflectivity of the probe laser beam was calibrated on two known values. The zero signal level corresponded to the reflectivity of Si at the room temperature, which was calculated from the data in Ref. 12. The maximum signal level for energy densities well above the melting threshold was determined by the reflectivity of the liquid phase, which was taken from Ref. 13. For each measurement, the maximum value of the reflectivity of the probe laser beam, $R^{\mathrm{P}}_{\mathrm{max},\,i}(E_i)$, was found. The error limit of the measurements of $R^{\mathrm{P}}_{\mathrm{max}}$ was ±1% in our setup. The results are shown in Fig. 1, where stars denote the experimental data.

The thermal model [10] was employed to calculate the $R^{\mathrm{P}}_{\mathrm{max,\,c}}(E)$ functions with the energy densities in the range $E \in [0.3\ \mathrm{J\cdot cm^{-2}}, 0.67\ \mathrm{J\cdot cm^{-2}}]$, which all were below the melting threshold of c-Si. All the thermodynamic input parameters of this model have been considered as

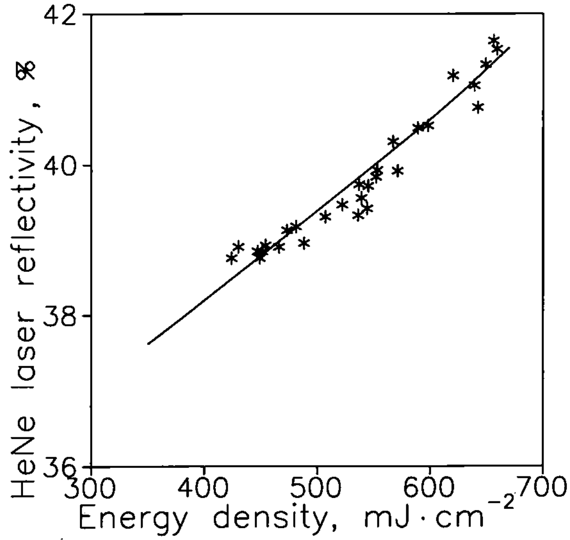

Fig. 1. Maximum reflectivity of monocrystalline silicon at the wavelength of the HeNe probe laser vs energy density of the XeCl laser pulse calculated using the values of $R_s(T)$ determined by the new fitting procedure (——). Stars denote experimental data.

temperature dependent. The application of the algorithm described in Section 2 resulted in the following expression for R_s: $R_s = 0.590 \pm 0.005 + (4.5 \pm 0.5) \times 10^{-5}(T - 293)$. This R_s function is shown as the solid line in Fig. 1; its agreement with the experimental data is very good. The tests of goodness of fit resulted here in a correlation coefficient $r = 0.99$.

Comparing the above expression for the reflectivity of solid silicon at 308 nm with the data published by other authors, we found that the results of our fitting procudure agree well with the corresponding relation from Ref. 14, which reads $R_s = 0.59 + 4 \times 10^{-5}T$.

The error analysis of the method for determining the temperature-dependent reflectivity of solid semiconductors described in Section 2 was performed in an empirical way, together with a similar analysis for its "parent" method developed in Ref. 9 for liquid semiconductors, since it is apparent that any error in the c-Si data must always be accompanied by errors in the quantities which are characteristic of the liquid state (such as the melt duration, the maximum thickness of the molten layer, etc.). Also, it is useful to compare the errors arising from the uncertainties of the parameters of the solid and the liquid phases.

First, we performed tests of the influence of uncertainty in the input parameters of the mathematical model on the accuracy of computed values of the maximum reflectivity of the probe laser, $R^{\mathrm{P}}_{\mathrm{max,\,c}}$, and the melt duration, $t_{\mathrm{m,\,c}}$. It was observed that the influence of errors in the parameters of liquid silicon (l-Si) was not much higher, despite their higher uncertainty (5%, on average), than that in the parameters of c-Si (typically, 0.5–1%). We observed the maximum error in $t_{\mathrm{m,\,c}}$ to be 2.1%, in $R^{\mathrm{P}}_{\mathrm{max,\,c}}$ even 0.1% which is due to the low thickness of the l-Si layer compared to the c-Si bulk and its relatively high thermal conductivity.

The influence of errors in the c-Si parameters was more important. The maximum errors in $t_{\mathrm{m,\,c}}$ were observed for energy densities just above the melting threshold but the 4.6% error represented here less than 1 ns. The accuracy of $R^{\mathrm{P}}_{\mathrm{max,\,c}}$ was higher, the maximum error being 1.7% in the "transition zone" (i.e., in the region where the liquid layer is still optically thin for the laser light and the resulting reflectivity of the liquid–solid system is somewhere between the hot–solid and the liquid values).

We also tested the influence of errors in the fitted parameters on the accuracy of the computed values of $R^{\mathrm{P}}_{\mathrm{max}}$ and t_{m}. Here the effect of the reflectivity of l-Si, $R_{\mathrm{l}} = R_{\mathrm{lo}} + B(T - T_{\mathrm{m}})$, where R_{lo} is the reflectivity of l-Si at the melting temperature T_{m}, B is a constant (see Ref. 9 for details), was generally more important. The most marked influence on the accuracy of computional results was exhibited by the coefficient B, i.e., by the slope of the R_{l} curve. The variation by 5% in B can result in a 4.2% change in $t_{\mathrm{m,\,c}}$

and a 2.3% change in $R^{\mathrm{P}}_{\mathrm{max,\,c}}$. Neglecting the temperature dependence of R_1 can decrease the value of $t_{\mathrm{m,\,c}}$ by more than 12%.

The influence of R_{10} on the computed quantities $R^{\mathrm{P}}_{\mathrm{max}}$, t_{m} is most important in the second part of the "transition zone" apparently, approximately for $E \in [0.75\ \mathrm{J \cdot cm^{-2}}, 0.95\ \mathrm{J \cdot cm^{-2}}]$. It was observed that a change of 1.5% in R_{10} can result in a 1.7% variation of $R^{\mathrm{P}}_{\mathrm{max,\,c}}$. Similarly, changing R_{10} by 3% results in a 10% difference if $R^{\mathrm{P}}_{\mathrm{max,\,c}}$.

The least influence was exhibited by variations in the coefficient A, i.e., in the slope of the $R_s(T)$ curve. Changing A by 5% led to a variation of only 0.3% in $R^{\mathrm{P}}_{\mathrm{max,\,c}}$. The influence of uncertainty in the thermodynamic parameters of our model on $R^{\mathrm{P}}_{\mathrm{max,\,c}}$ is, in the range of energy densities which are of interest in this case, i.e., $E \in [0.30\ \mathrm{J \cdot cm^{-2}}, 0.65\ \mathrm{J \cdot cm^{-2}}]$, also very low, not exceeding 0.15%, and as mentioned before, the correlation with the experimental data is very high.

4. CONCLUSION

The combined experimental and numerical method for determining the reflectivity of solid semiconductors in dependence on temperature developed in this paper is very fast compared to the standard methods such as scanning ellipsometry. In addition, the error analysis of this method has shown that its precision is quite sufficient for common applications. Therefore, the method can be considered as a useful tool for obtaining fast information on the dependence of reflectivity on temperature, although it cannot replace the well-established methods, which are generally more universal and do not need complementary data. In addition, the new method can be successfully combined with the data obtained by some classical method at room temperature if a fast information is required.

Numerical tests of the method described in this paper and of its "parent" method for liquid semiconductors developed in Ref. 9 revealed that the precision of thermodynamic parameters of the solid phase and of the slope of the $R_1(T)$ curve are the most important factors influencing the accuracy of calculated values of the characteristic parameters of laser processing and, consequently, also the accuracy of both the combined methods for determining reflectivity of semiconductors presented in Ref. 9 and here.

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