THERMAL FIELDS IN FILM MICROELECTRONIC STRUCTURES ON EXPOSURE TO RADIATION HEATING

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A model of heating of film structures by incoherent light is presented and results of numerical experiments are reported on the investigation of thermal fields for the cases of a dielectric film that is transparent to radiation and an absorbing metal film on silicon.

High-speed heat processing of microelectronic structures with the use of intense radiation fluxes looks promising for the formation of silicide layers on semiconductor substrates and metallization systems, and also for improving the quality of dielectric films and the boundary surface between semiconductor and dielectric [1, 2]. In this case the temperature fields attained in heterogeneous layered structure are determined both by the properties of the constituent materials and the parameters of the radiation used [3-6]. Experimental recording of these fields is difficult; therefore, their theoretical simulation is of current interest.

Simulation of the heating of the film structure calls for consideration of different spectral and thermal dependencies of optical and thermophysical parameters of film and substrate materials and also features of the distribution of the heat energy liberated in such a structure. Specificity of real film structures results in the appearance of additional terms in the balance of the supplied energy. The main effects that should be taken into account are: (1) radiation flux on the inner boundaries of absorbing, radiating, and scattering media [7, 8], when radiation properties of the adjacent films (or the film and substrate) are different; (2) an increase in the transmission coefficient in the region of transparency of a semiconductor substrate (by 10-30%) with a dielectric film on its surface, which improves transparency due to interference effects on the boundary surface [9, 10]; and (3) liberation (absorption) of the latent heat of phase transition w_r.

The last-mentioned process can be considered instantaneous under conditions of high-speed thermal processing of thin-film structures. However, in the general case it depends on the film thickness and on the temperature gradients that arise during heating.

The assumption of homogeneity of the irradiation of the sample along the entire surface and the condition of the geometrical dimensions of the irradiated surface being considerably larger than the thickness of the sample allow one to restrict consideration to the one-dimensional case.

We assume that the structure consists of $n - 1$ films (Fig. 1), each of which ($1 \leq j < n$) is $Z_{j+1} - Z_j$ in thickness, and its material is characterized by the density ρ_j, specific heat C_j, and also by the coefficients of reflection R_j, absorption α_j, and heat conduction K_j. In such notation, parameters with the index $j = n$ refer to the substrate.

The distribution of the temperature $T_j = T_j(Z, t)$ in the film structure is obtained by numerical solution of the system of nonlinear heat equations of the form

$$\frac{\partial T_j}{\partial t} = \frac{1}{C_j \rho_j} \left\{ \frac{\partial}{\partial Z} \left[K_j(T_j) \frac{\partial T_j}{\partial Z} \right] + A_j(Z_j < Z < Z_{j+1},\ T_j,\ t) \right\}, \quad (1)$$

written for each film ($j = 1, 2, \ldots, n - 1$) and the substrate ($j = n$).

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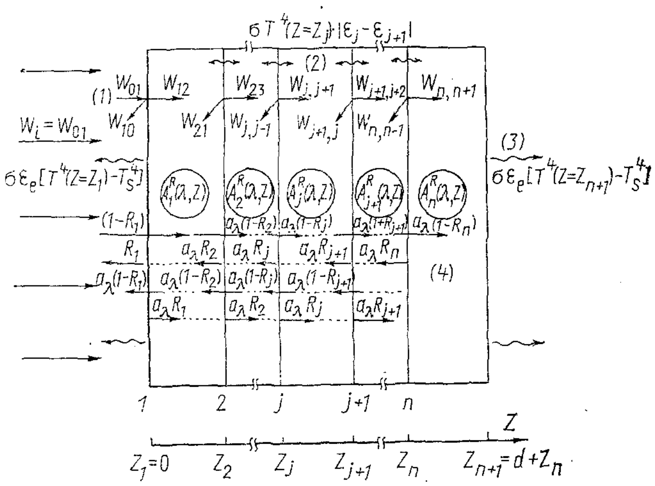

Fig. 1. One-sided heating of the film structure by an extensive radiation flux.

In this case the following boundary conditions are used:

$$-K_1(T_1)\frac{\partial T_1}{\partial Z}\Big|_{Z=Z_0}+\sum_{i=t,c} w_i(T_1)=0; \tag{2}$$

$$K_n(T_n)\frac{\partial T_n}{\partial Z}\Big|_{Z=Z_{n+1}}+\sum_{i=t,c} w_i(T_n)=0, \tag{3}$$

which take account of heat exchange due to radiation $w_t = \sigma\varepsilon_e(T^4_{sub} - T^4_{sur})$ and convection $w_c = \alpha_c(T_{sub} - T_m)$, and also conditions of discontinuity of the heat flux and equality of temperatures on both sides of interlayer boundaries ($1 < j < n$) taking account of energy expenditure in phase transitions:

$$K_j\frac{\partial T_j}{\partial Z}\Big|_{Z=Z_{j+1}}=K_{j+1}\frac{\partial T_{j+1}}{\partial Z}\Big|_{Z=Z_{j+1}}+w_r(T_j), \tag{4}$$

$$T_j(Z_{j+1})=T_{j+1}(Z_{j+1}). \tag{5}$$

With account for redistribution of radiation energy in the inner surfaces, the portion of light energy absorbed in the j-th film can be represented in the form

$$A_j^R(\lambda,\ Z_j\leqslant Z\leqslant Z_{j+1})=W_{j,j+1}a_e(Z_j,\ Z)+W_{j+1,j}a_e(Z,\ Z_{j+1}), \tag{6}$$

where the parameter of heat generation

$$a_e(Z,\ Z_j)=\exp\Big[-\int\limits_{Z}^{Z_j}\alpha(Z')\,dZ'\Big]; \tag{7}$$

$\alpha(Z')$ is a piecewise-continuous function constructed from partial $\alpha_j(\lambda, T)$ for the entire film structure. We write the corresponding parts of the radiation transmitted ($j < k$) or reflected ($j > k$) on the j-th boundary $W_{j,k}$ in the form

$$W_{0,1}=W_I; \tag{8}$$

$$W_{j,j+1}=W_{j-1,j}(1-R_j)+W_{j+1,j}a_e(Z_j,Z_{j+1})R_j; \tag{9}$$

$$W_{j+1,j}=W_{j,j+1}a_e(Z_j,Z_{j+1})R_{j+1}+W_{j+2,j+1}a_e(Z_{j+1},Z_{j+2})(1-R_{j+1}); \tag{10}$$

$$W_{j+1,j+2}=W_{j,j+1}a_e(Z_j,\ Z_{j+1})(1-R_{j+1})+W_{j+2,j+1}a_e(Z_{j+1},\ Z_{j+2})R_{j+1}; \tag{11}$$

$$W_{j+2,j+1}=W_{j+1,j+2}a_e(Z_{j+1},\ Z_{j+2})R_{j+2}. \tag{12}$$

With the use of Eqs. (7)-(12), the generalized expression for the internal source of heat by analogy with the expression obtained in [11] for the radiation heating of substrates, homogeneous in thickness, in the case under consideration assumes the form

TABLE 1. Dependencies of Thermophysical and Optical Parameters of Layers, Used in Thermal Calculations of Silicon-Based Film Structures

Parameter	Material	
	SiO_2	Al
Density (ρ), g/cm^3	2,20 [12]; 2,1—2,2 [13]; 2,22 [14]	2,70 [15, 16]; 2,38, 660°C [16]
Melting point (T_{mp}) K	1893 [15]; 2073 [14]	933,65 [17]
Coefficient of thermal conductivity (K(T)), W/(cm·K)	$34/(T-234\ K)$ [18]; $2\cdot 10^{-3}T^{0,336}$, $300<T<696$ K; $2,3\cdot 10^{-6}T^{1,37}$, $696<T<1149$ K [5]; $7,3\cdot 10^{-11}T^{2,84}$, $T>1149$ K	4,23, 933 K [16]; 1,04, 973 K [16]
Specific heat ($c_p(T)$) J/(g·K)	$931,3+0,256T-24,0\cdot 10^6 T^{-2}$; $300<T<2000$ K [12]	0,92 [15]; $0,90+4,19\cdot 10^{-4}(T-300\ K)$ [15]
Forbidden band width (E_g), eV	8,1 [13]	—
Coefficient of photon absorption (α)	$\alpha_\lambda(d)\approx(1-5)\%$ [19, 20]; $\alpha(SiO_2)/\alpha(Si)\lesssim 10^{-2}$ [15, 21]	$8,0\cdot 10^4\ cm^{-1}$ [22]
Coefficient of photon reflection (R)	$\lesssim 0,2$ [23]; $\simeq 0,05-0,10$, $T=300$ K [20]	0,89 [15]; 0,77 [20]

$$A(Z,\ T,\ t)=\frac{W_I\,(1-R_1-\tau^*(T,\ d))\,f(t,\ \tau_p)\int\limits_{\lambda_1}^{\lambda_2} I(\lambda,\ T_h)\,\alpha(\lambda,\ T)\,A^R(\lambda,\ Z)\,d\lambda}{\int\limits_{Z_1}^{Z_4} dZ\int\limits_{\lambda_1}^{\lambda_2} I(\lambda,\ T_h)\,\alpha(\lambda,\ T)\,A^R(\lambda,\ Z)\,d\lambda}. \tag{13}$$

The proposed description of processes of heat liberation in film stuctures heated by radiation takes account of spectral composition, thermal and spectral dependencies of optical and thermophysical parameters of the semiconductor substrate and films on its surface when specifying inner source of heat, while possible energy losses on thermal radiation, convection, and phase transformations are taken account of in the boundary conditions. The latter allows one to investigate the influence of chemical reactions, initiated by heating (among which are oxidation, nitriding, silicide formation, etc.) in microelectronic structures, on the heat balance. Calculations with the use of the above expressions are realized with the help of numerical methods.

Calculations are performed for two typical microelectronic structures: a dielectric film that is transparent to radiation, and an absorbing metal film on a silicon substrate, with account for dependencies of optical and physical parameters of these materials, generalized in Table 1.

We consider the structure represented by a silicon slice, on the surface of which are formed successively films of silicon dioxide and polycrystalline silicon, subject to heating by incoherent light.

When calculating numerically temperature distributions T = T(Z, t) along the width of this structure, we used the system of heat equations of the form (1) with boundary conditions (2), (3), and coupling conditions (4) and (5). In addition, we took account of radiation heat exchange on inner boundaries.

The fraction of light energy absorbed by a thin film of polycrystalline silicon was determined from the equation

$$A_1^R(\lambda,\ Z_1\leqslant Z\leqslant Z_2)=W_{1,2}a_e(Z_1,\ Z)+W_{2,1}a_e(Z,\ Z_2), \tag{14}$$

obtained from (6) for n − 1 = 3. Here

$$W_{1,2}=W_{0,1}(1-R_1)+W_{1,2}a_e(Z_1,\ Z_2)\ R_1; \tag{15}$$

$$W_{2,1}=W_{1,2}a_e(Z_1,\ Z_2)R_2+W_{3,2}(1-R_2); \tag{16}$$

$$W_{3,2}=W_{2,3}R_3; \tag{17}$$

$$W_{2,3}=W_{1,2}a_e(Z_1,\ Z_2)\ (1-R_2)+W_{3,2}R_2. \tag{18}$$

On the other hand, for the fraction of energy absorbed by a translucent silicon substrate, we can apply the expression

$$A_3^R(\lambda,\ Z_3 \leqslant Z \leqslant Z_4) = W_{3,4} a_e (Z_3,\ Z). \tag{19}$$

Hence, by using Eqs. (15)-(18) for the components playing a decisive role in calculations, we obtain

$$W_{1,2} = W_{0,1}(1 - R_1)/(1 - \vartheta); \tag{20}$$

$$W_{2,1} = W_{1,2}\vartheta / a'_e R_1; \tag{21}$$

$$W_{3,4} = W_{1,2} a'_e (1 - R_2)(1 - R_3)/(1 - R_2 R_3), \tag{22}$$

where the parameter $\vartheta = (a_e')^2 R_1[R_2 + R_3(1 - 2R_2)]/(1 - R_2R_3)$, and $a_e' = a_e(Z_1,\ Z_2)$.

Since functions K(T) and A(Z, T, t) were piecewise continuous, we used a balance method [24] when constructing a difference scheme, and a special scheme, for which the available discontinuity points were nodal. The generalized solution obtained by the pivotal method is unique and stable in the range of the parameters that we used. Iterations were used to resolve the existing temperature nonlinearities. At the same time, if the number of necessary iterations for the simulation of thermal fields in structures with a single point does not exceed 4, then for the calculations of multiple-film structures we require 5-8 iterations.

In Fig. 2, the calculated temperature of the irradiated surface of the structure under consideration is represented as the dependence on the exposure density of radiant power of haloid incandescent lamps for the duration of exposure equal to 15 sec, and also a profile of temperature distribution along the thickness of the structure for power densities equal to 35 W/cm^2. It seems interesting to compare calculations of the fraction of light energy absorbed by a single-crystal silicon slice (~9%), polycrystalline silicon film (~20%), and also reflected in the surrounding medium (~71%) when the investigated structure is irradiated from the direction of the film.

The exhibited temperature gradients are not high – for a silicon slice 380 μm in thickness, $\Delta T \sim 15°$ when heated from the direction of the surface with films and $\Delta T \sim 7°$ when heated from the reverse direction, the temperature of the silicon slice being considerably higher than the temperature of the film structure when heated from the direction of the film surface; and it exceeds by 250°C the temperature of such a structure when heated from the direction of the substrate. Therefore, the presence of several films on the slice surface, transparent or translucent to radiation, modifies substantially its heating regime.

For the radiant heating of a microelectronic structure with a metal film on the surface of a semiconductor substrate, the value of the reflection coefficient affects substantially the heating regime. As our calculations for silicon slices with films of aluminum, gold, platinum, and vanadium formed on their surfaces have shown, the temperature induced during the heating of such a structure can decrease by a factor of four as compared with the temperature attained by irradiating these structures from the direction of the substrate.

Thus, in the heating of the structure aluminum film/silicon for a few seconds, the efficiency of heating for irradiation from the direction of the metal film (Fig. 3) decreases by a factor of 2-2.5 (in absolute value of the induced temperature). When heated from the direction of the semiconductor substrate without a film, the efficiency of heating as compared with the free substrate increases by 18-20% (Fig. 3).

Calculations of the thermal fields of silicon-based film structures, exposed to radiant heating, performed with the use of the developed model, allow us to conclude that it is advisable to conduct heat processing of such structures from the direction of the film-free substrate surface, which increases the efficiency of utilization of the exposure energy.

The proposed description of thermal processing of semiconductor structures allows us to simulate thermal regimes, realized in experimental set-ups, taking account of the features of film structures.

NOTATION

d, substrate thickness; τ_p, duration of the radiant pulse; Z, coordinate; t, time; λ, radiation wavelength; W_I, exposure density of the irradiating power; $f(t, \tau_p)$, its dependence on time; $I(\lambda, T_h)$, spectral distribution of the radiation intensity; T_h, chromatic temperature; τ^*, integral transmission coefficient; ε_e, radiating capacity of the system of sample-heating chamber; σ, Stefan–Boltzmann constant; α_c, coefficient of convective heat

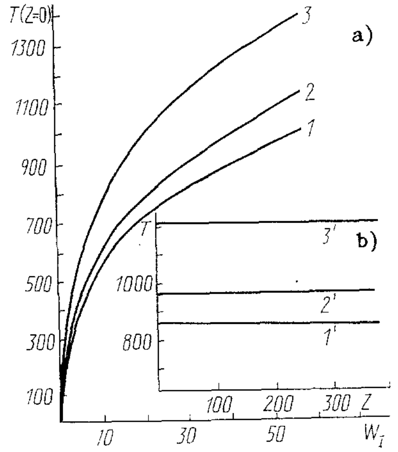

Fig. 2

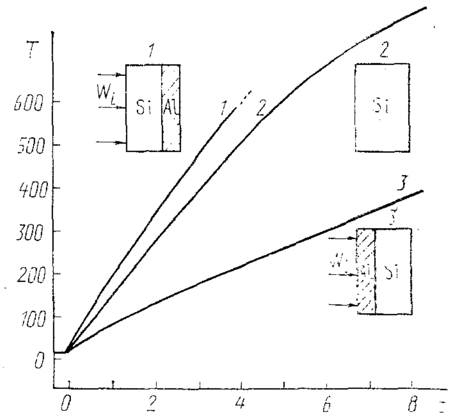

Fig. 3

Fig. 2. (a) Dependence of the temperature of the irradiated surface (film structure: polysilicon/silicon dioxide/silicon) on the density of a radiation pulse; (b) temperature distribution during heating (W_I = 35 W/cm^2) from the direction of the film (1, 1'), from the reverse direction (2, 2'), and silicon slice without filsm (3, 3'). T, °C; W_I W/cm^2; Z, μm.

Fig. 3. Dependence of the temperature of the structure aluminum film/silicon on the duration of exposure to an incoherent light pulse (W_I ~ 14 W/cm^2) from the direction of the substrate (1); from the direction of the metal film (3); in the process of irradiation of a silicon slice, free of films (2). T, °C; t, sec.

dissipation; T_{sub}, T_{sur}, and T_m, the temperatures of the substrate, surrounding surfaces, and surrounding media, respectively.

LITERATURE CITED

1. V. A. Labunov et al., Zarub. Élektr. Tekh., No. 8, pp. 27-53 (1985).
2. A. S. Smul'skii et al., Élektr. Tekh. Ser. 2. Semiconductor Devices, No. 5(156), 78 (1985).
3. P. Baeri, S. U. Campisano, M. G. Grimaldi, and E. Rimini, J. Appl. Phys., 53, No. 12, 8730-8733 (1982).
4. P. K. Bhattacharya, S. K. Gupta, and A. G. Wagh, Radiat. Eff., 63, No. 5, 197-204 (1982).
5. K. Kubota, C. E. Hunt, and J. Frey, Appl. Phys. Lett., 46, No. 12, 1153-1155 (1985).
6. M. A. Korolev, S. G. Tadevosyan, V. A. Khaustov, Élektron. Tekh. Ser. 3. Mikroélektronika. No. 2(122), 58-60 (1987).
7. A. S. Okhotin et al., Heat Conduction in Solids. Handbook [in Russian], Moscow (1984).
8. E. M. Sparrow and R. D. Cess, Radiation Heat Transfer, McGraw-Hill (1978).
9. P. Baeri, G. Foti, and J. M. Poate, J. Appl. Phys., 50, No. 5, 3783-3792 (1979).
10. J. P. Colinge and F. Van de Wiele, J. Appl. Phys., 52, No. 7, 4769-4771 (1981).
11. V. E. Borisenko et al., Phys. Status Solidi (1), 86, No. 2, 573-583 (1984).
12. O. A. Sergeev and A. G. Shashkov, Thermophysics of Optical Media [in Russian], Minsk (1983).
13. E. I. Shnarevich, O. A. Rybinskii, and V. A. Zlobin, Dielectrics in Integrated Circuits [in Russian], Moscow (1975).
14. D. J. Godfrey, A. C. Hill, and C. Hill, J. Electrochem. Soc. 128, No. 8, 1798-1803 (1981).
15. I. K. Kikoin (ed.), Tables of Physical Quantities, Handbook [in Russian], Moscow (1976).
16. L. V. Gurevich, I. V. Veits, and V. A. Medvedev, Thermodynamical Properties of Individual Substances, Handbook [in Russian], Moscow (1978).

17. V. A. Ryabin, Thermodynamical Properties of Substances [in Russian], Leningrad (1977).
18. A. Lietoila, Laser Processing of High-Dose Ion Implanted Si: The Solid Phase Regime, Thesis, Stanford (1981), p. 120.
19. A. E. Sheindlin (ed.), Radiation Properties of Solids, Handbook [in Russian], Moscow (1974).
20. D. B. Zvorykin and Yu. I. Prokhorov, Application of Radiant Infrared Heating in Electronic Engineering [in Russian], Moscow (1980).
21. A. S. Okhotin and A. S. Pushkarskii, Thermophysical Properties of Semiconductors [in Russian], Moscow (1972).
22. C. W. White and P. S. Peercy (eds.), Laser and Electron Beam Processing of Materials, New York (1980), pp. 6-9.
23. A. Bhattacharya, B. G. Streetman, and K. Hess, J. Appl. Phys., 52, No. 5, 3611-3617 (1981).
24. N. M. Belyaev and A. A. Ryadno, Methods of the Theory of Heat Conduction [in Russian], Moscow (1982).

POWER-LAW APPROXIMATION OF TRANSFER FUNCTION IN NONSTEADY HEAT- AND MASS-TRANSFER PROBLEMS

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A power-law approximation of the transfer function for heat- and mass-transfer problems is proposed, enabling the temperature at a fixed point to be found to within 2%.

The method of imaginary-frequency characteristics (IFC) proposed in [1] and developed for heat- and mass-transfer problems in [2, 3] consists in replacing the accurate transform F(p) in the region of real p by some approximate function Φ(p), the inverse of which may readily be found. It was shown in [1] that, for weakly oscillatory systems, the error of the inverse is practically equal to the error of the approximation of the transform. In [3], the IFC method was used to construct analytical solutions of the thermal-conductivity problems for an infinite plate, cylinder, and sphere. The accuracy of the results is 1-3%. However, the use of piecewise-rational functions for Φ(p) in [3] leads to certain difficulties in finding the coefficients of the approximation [4]. Therefore, the question of using functions of a different form for this purpose arises. Investigations show that, for monotonic dependences F(p) such as the transfer functions in heat- and mass-transfer problems, a sufficiently effective approximation is a power-law function

$$\Phi(p)=\left(\frac{A}{A+p}\right)^{L}\exp(-Tp). \tag{1}$$

In comparison with the piecewise-rational function, this approximation permits more effective description of both slowly and rapidly decreasing dependences. In addition, the parameters A, L, T in [1] may be found by the least-squares method, which leads to fairly complex nonlinear expressions in the case of the piecewise-rational function [1].

The scheme of the least-squares method for the case of [1] is now outlined. Suppose that F(p) is normalized to F(0) = 1, and its value is known at N points. Then, the parameters of the approximation are found from the condition of a minimum of the sum of squares of the deviations of ln F(p) and ln Φ(p)

$$Q=\sum_{i=1}^{N}\left[\ln F(p_i)-L\ln\frac{A}{p_i+A}+Tp_i\right]^2\rightarrow\min. \tag{2}$$

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