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HEAT EXCHANGE BETWEEN A SUBSTRATE AND SUBSTRATE HOLDER IN THERMAL CONTACT

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The article presents the results of an experimental investigation of high-temperature contact heat exchange between the polished surface of a substrate and the rough surface of a substrate holder under various conditions of contact between them in different gas media, under vacuum, and at different gas flow rates.

Introduction. The processes of chemical deposition of monocrystalline layers of semiconducting materials from the gas phase onto monocrystalline substrates are among the basic processes in the production of active elements of integrated circuits.

Substrates are mounted in a polyhedral prismatic substrate holder heated in a reaction chamber to operating temperature. The uniformity of the substrate temperature, which is determined by the conditions of its contact with the substrate holder surface, ensures that high-quality structures are formed in the deposited layer.

The reliability of thermal contact between contacting items can be ensured by increased specific loads or by materials (adhesives, pastes, mastics) that fill the gap between them and have a relatively high thermal conductivity coefficient [1].

However, the extremely high requirements to the cleanliness of semiconductor fabrication and the low mechanical strength of the substrate material preclude the above-mentioned recommendations. This was the reason for the carrying out the present investigation.

Investigation Procedure. We consider one of the typical cases of mounting of substrates on a substrate holder, when thermal contact between them is ensured by the weight of the substrate itself. For example, a silicon substrate of thickness $\delta_s = 0.4$ mm and diameter $d_s = 100$ mm weighs about 8 g.

A diagram of thermal contact between a substrate and its holder and the temperature variation in the "substrate holder–substrate–wall of reaction chamber" system are presented in Fig. 1. The same figure (at the left) also shows (in scale) a fragment of the recorded surface waviness of a typical substrate holder.

The roughness of the substrate holder surface and the waviness of the substrate lead to the appearance of a gap between them Δ whose thickness is much smaller than the substrate diameter d_s, i.e., $d_s >> \Delta$.

Let us set up a heat balance equation for the system analyzed. The heat flux supplied from the holder to the substrate is

$$q_1 = q_{r1} + q_{tg} + q_{tdc} . \quad (1)$$

The heat flux transferred by the substrate to the reaction chamber walls is

$$q_2 = q_{r2} + q_c . \quad (2)$$

Let us write expressions for the heat fluxes in terms of their components:

$$q_{r1} = \alpha_{r1} (T_{sh} - T_{s1}) = \varepsilon_{red1}\sigma_0 \left[\left(\frac{T_{sh}}{100}\right)^4 - \left(\frac{T_{s1}}{100}\right)^4 \right] , \quad (3)$$

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$$q_{tg} = \left(\frac{\lambda_g}{\Delta^*}\right)_g (T_{sh} - T_{s1}) , \tag{4}$$

$$q_{tdc} = \left(\frac{\lambda_{sh}}{\Delta^*}\right)_{dc} (T_{sh} - T_{s1}) , \tag{5}$$

$$q_{r2} = \alpha_{r2} (T_{s2} - T_w) = \varepsilon_{red2}\sigma_0 \left[\left(\frac{T_{s2}}{100}\right)^4 - \left(\frac{T_w}{100}\right)^4\right] , \tag{6}$$

$$q_c = \alpha_c (T_{s2} - \overline{T}_g) . \tag{7}$$

Here ε_{red1} and ε_{red2} are the reduced emissivities of the systems: "substrate holder–substrate" (system 1) and "substrate–reaction chamber wall" (system 2), respectively; T_{sh}, T_{s1}, T_{s2}, T_w are the temperatures of the substrate holder, of the side of the substrate facing the holder, of the side of the substrate facing the reaction chamber wall, and of the reaction chamber wall; $\overline{T}_g$ is the mean temperature of the gas contained between the substrate and the reaction chamber wall; λ_g and λ_{sh} are the thermal conductivity coefficients of the gas and of the substrate holder material, respectively; $\sigma_0 = 5.67 \cdot 10^{-8}$ W/m^2 K^4 is the Stefan–Boltzmann constant; α_{r1}, α_{r2}, α_c are the radiative heat transfer coefficients of systems 1 and 2, and the coefficient of heat transfer by convection from the substrate to the gas flow, respectively.

The radiative heat transfer coefficient of system 1 is

$$\alpha_{r1} = \varepsilon_{red1}\sigma_0 (T_{sh}^3 + T_{sh}^2 T_{s1} + T_{sh} T_{s1}^2 + T_{s1}^3) . \tag{8}$$

The reduced emissivity $\varepsilon_{red\,1}$ can be determined from the expression for a system of plane-parallel bodies, since

$$\varepsilon_{red1} = \frac{1}{\dfrac{1}{\varepsilon_s} + \dfrac{1}{\varepsilon_{sh}} - 1} . \tag{9}$$

Since for the substrate the number Bi << 1, then with an accuracy sufficient for calculation we may write

$$T_{s1} \approx T_{s2} = T_s .$$

The substitution of Eqs. (3)-(5) into Eq. (1) on the assumption that the resulting heat flux components do not influence one another, leads to the equation

$$q_1 = \left[\alpha_{r1} + \left(\frac{\lambda_g}{\Delta^*}\right)_g + \left(\frac{\lambda_{sh}}{\Delta^*}\right)_{dc}\right] (T_{sh} - T_s) = \frac{1}{R_1} (T_{sh} - T_s) . \tag{10}$$

The substitution of Eqs. (6) and (7) into Eq. (2) yields

$$q_2 = (\alpha_{r2} + \alpha_c) (T_s - T_w) = \frac{1}{R_2} (T_s - T_w) . \tag{11}$$

Under the conditions of a steady-state heat regime the following equality holds

$$q_1 = q_2 = q_{res} . \tag{12}$$

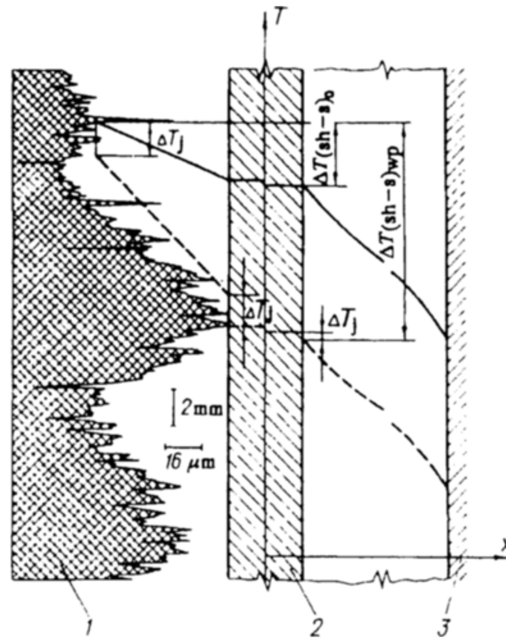


Fig. 1. Computational model of "substrate (2)–substrate holder (1)–reaction chamber wall (3)" system with a fragment of recorded profile (in scale) of substrate holder surface (cross-hatched region).

Taking into account Eq. (12) and proceeding from Eqs. (10) and (11), let us write an expression for the temperature difference between the substrate holder and the reaction chamber wall:

$$T_{sh} - T_w = (R_1 + R_2)\, q_{res} \,. \tag{13}$$

In the case of a fixed value of q_{res} and changing pressure in the reaction chamber, the temperature difference between the substrate holder and the reaction chamber wall $(T_{sh} - T_w)$ is preserved constant. But the temperature difference between the substrate holder and substrate $(T_{sh} - T_s)$ changes with the size of the gap and conditions of contact between them, the total pressure in the reaction chamber (in the case when the number Kn > 0.01 [2]), and the heat flux direction. Consequently, the thermal state of the substrate will be determined by the value of $\Delta T = T_s - T_{sh}$. In the case of induction heating the temperature of the substrate holder is higher than that of the substrate, i.e., the latter is underheated and $\Delta T < 0$. In the case of radiant infrared heating the temperature of the substrate exceeds that of the holder and $\Delta T > 0$.

It is advisable to represent the results of investigation of the effect of the total pressure in the reactor on the thermal state of the substrate in a general form. The unknown parameter of the system is selected to be the relative magnitude of "underheating" ("overheating") of the substrate:

$$\Theta = \frac{(T_{sh} - T_s)_{wp}}{(T_{sh} - T_s)_0} = \frac{\left(1 + \dfrac{R_2}{R_1}\right)_0}{\left(1 + \dfrac{R_2}{R_1}\right)_{wp}} \,, \tag{14}$$

which is the ratio of the value of $(T_{sh} - T_s)_{wp}$ under the investigated (working) pressure to the value of $(T_{sh} - T_s)_0$ at atmospheric pressure. The value of the relative pressure $\overline{P} = P/P_0$ was selected as a determining parameter.

To calculate the thermal conductivity of the gap, it is necessary to know the size of the effective gas interlayer Δ^*. The asterisk is used because the size of the gas interlayer between the points of direct (physical)

contact of the substrate with its holder changes, since the substrate holder surface is rough and has grooves of various depths (see Fig. 1).

We will determine the thermal conductivity of a direct contact assuming that this value is independent of both the total pressure in the reaction chamber and the type of gas. For this purpose, it is sufficient to change the composition of the gas medium that fills the reaction chamber, for example, to carry out investigations in a medium of hydrogen and in a medium of argon, whose thermal conductivity coefficient is smaller by an order of magnitude. Then, it is necessary to set up and solve a system of equations that include components for heat conduction through direct contact and gas interlayers.

When the reaction chamber is filled with hydrogen,

$$\left[\left(\frac{\lambda_g}{\Delta^*}\right)_g + \left(\frac{\lambda_{sh}}{\Delta^*}\right)_{dc}\right] \Delta T_{0H_2} = (q_{tg} + q_{tdc})_{0H_2} \tag{15}$$

and with argon,

$$\left[\left(\frac{\lambda_g}{\Delta^*}\right)_g + \left(\frac{\lambda_{sh}}{\Delta^*}\right)_{dc}\right] \Delta T_{0Ar} = (q_{tg} + q_{tdc})_{0Ar} . \tag{16}$$

The values of the quantity $(q_{tg} + q_{tdc})$ for a medium of hydrogen and that of argon can be determined if we know the values of q_{r1}, q_{r2}, and q_{res}. The values of q_{r1} and q_{r2} are easily calculated by formulas (3) and (5), and the value of q_{res} can be found experimentally.

Equations (15) and (16) make it possible to calculate the thermal conductivities of direct contact between the substrate and its holder.

For hydrogen

$$\left(\frac{\lambda_{sh}}{\Delta^*}\right)_{dc} = \left(\frac{q_{tg} + q_{tdc}}{\Delta T_{H_2}} - \frac{\lambda_{H_2}}{\Delta^*}\right)_0 = \left[\left(\frac{q}{\Delta T}\right)_{H_2} - \frac{\lambda_{H_2}}{\Delta^*}\right]_0 , \tag{17}$$

For argon

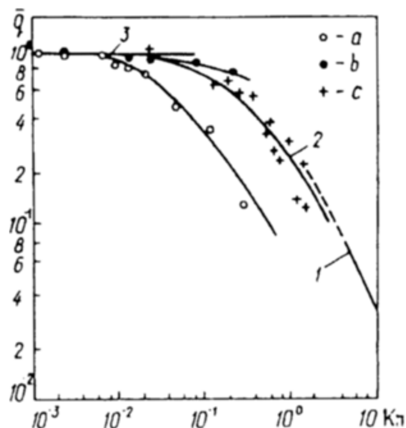
$$\left(\frac{\lambda_{sh}}{\Delta^*}\right)_{dc} = \left(\frac{q_{tg} + q_{tdc}}{\Delta T_{Ar}} - \frac{\lambda_{Ar}}{\Delta^*}\right)_0 = \left[\left(\frac{q}{\Delta T}\right)_{Ar} - \frac{\lambda_{Ar}}{\Delta^*}\right]_0 . \tag{18}$$

Since the left-hand sides of Eqs. (17) and (18) are equal to each other, the right-hand sides are also equal. After simple transformations we obtain equations for the size of the effective gas interlayer

$$\Delta^* = \frac{\lambda_{H_2} - \lambda_{Ar}}{\left(\frac{q}{\Delta T}\right)_{H_2} - \left(\frac{q}{\Delta T}\right)_{Ar}} . \tag{19}$$

Thus, to determine the values of Δ^* and Θ in investigations, it is necessary to measure the values of ΔT_{0H_2}, ΔT_{0Ar}, T_{sh}, T_s, and q_{res} and calculate the values of q_{tg} and q_{tdc} in a medium of hydrogen and that of argon.

Description of an Experimental Apparatus. We carried out all the investigations in the reactor of a UNES-2PK-A industrial apparatus for growing epitaxial layers of silicon [3]; the apparatus was reequipped for conducting processes at a reduced pressure. In order to maintain the normal operating conditions of the apparatus, a regulating throttle and an admission valve for inert gas were installed before the entrance to the reaction chamber to effect a smooth change in pressure from atmospheric to the prescribed degree of rarefaction. The pressure and rarefaction in the reaction chamber were controlled by an MOSh1-160 standard pressure gauge and a VO vacuummeter calibrated for 400 Pa and 260 Pa, respectively.



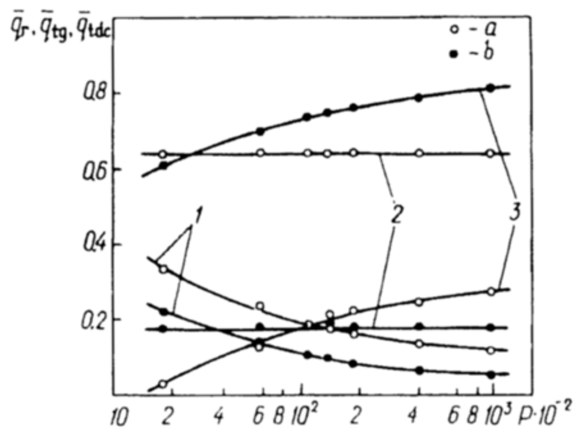


Fig. 2. Dependence of intensity of heat exchange of a layer of a stationary gas enclosed between parallel walls on the degree of rarefaction (Knudsen number): 1, 2, 3) calculated dependences for air in free molecular, molecular-viscous, and viscous (continuous) media [9]. Experimental points: a) argon; b) hydrogen; c) air [9].

Fig. 3. Effect of gas rarefaction degree on components of resultant heat exchange between substrate and substrate holder: 1) radiant component $\bar{q}_r$; 2) direct contact component $\bar{q}_{tdc}$; 3) component of heat conduction in gas interlayer q_{tg}; a) argon; b) hydrogen. P, Pa.

To measure the temperature difference between the substrate holder and the substrate located on its surface, we used an ÉOP-66 standard optical pyrometer. The pyrometer, which was calibrated beforehand using graphite samples with thermocouples imbedded in them, was installed on a stand. The design of the stand made it possible to measure the temperature distribution (through viewing quartz windows in the reaction chamber) over the height of the substrate holder.

The temperature control points of the substrate holder and substrate surfaces were close to one another.

The temperature of the substrate holder and substrate surfaces, which was maintained at a level of 1100–1200°C was measured with a maximum absolute error not exceeding ±6°C.

Calorimetry of the reaction chamber, which was carried out with the power of the induction heater stabilized, was used to determine the specific density of the resultant heat flux $q_{res} = 153 \cdot 10^3$ W/m^2.

We investigated two versions of substrate mounting on the holder: 1) the substrate contacted the holder surface under its own weight and 2) the substrate was separated by a distance of 3 mm from the holder surface by a graphite ring.

We carried out all the investigations with stationary and moving gases. This made it possible to estimate the effect of convective cooling of the substrate by gas flow.

Results and Their Discussion. The size of the effective gas interlayer $\Delta^* \approx 60$ μm was calculated from the measured values of ΔT_{OH_2}, ΔT_{OAr}, T_{sh}, T_s, and q_{res}, as well as from handbook data for the thermal conductivity coefficients of the gases [4] and the emissive characteristics of silicon and graphite [5, 6].

From the value of Δ^* we determined the specific densities of the heat fluxes transmitted by conduction to the gas interlayer q_{OH_2} and q_{OAr} and by direct contact of the substrate holder with the substrate in hydrogen $(q_{tdc})_{H_2}$ and argon (q_{tdc}). The resulting values in dimensionless form made it possible to determine the boundary of transition from a viscous (continuous) to a molecular-viscous medium.

Figure 2 presents calculated and experimental dependences of the heat transfer intensities in a stationary gas layer (H_2, Ar and air) enclosed between plane surfaces. The measure of intensity is the ratio of the specific densities of the heat flux transmitted by the conduction of the gas in the case of rarefaction q_{wp} and at atmospheric pressure q_0. Inspection of the figure shows that at a Kn number close to 0.01 the value of $\bar{q} = q_r/q_0$ deviates from unity, i.e., there occurs a transition to the molecular-viscous regime. Moreover, we note that, compared with argon,

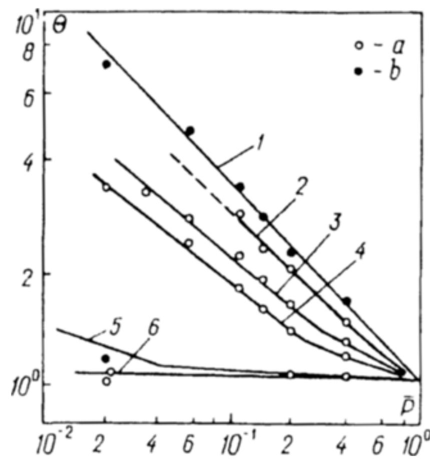


Fig. 4. Change in the relative temperature difference Θ between substrate and substrate holder versus the pressure in the reaction chamber $\bar{P}$ for different gas flow rates V_g and means of contact between substrate and its holder: 1) V_g = 2 m^3/hr; 2) 2.5; 3) 0.9; 4, 6) 0; 1-4) substrate lies on the holder; 6) substrate is separated from the holder surface by a distance of 3 mm; 5) data of [9]; a) argon; b) hydrogen.

the onset of transition from a continuous viscous to a molecular-viscous medium in hydrogen is displaced to the side of higher values of Kn numbers. This difference seems to be connected with a higher coefficient of accommodation of hydrogen in the silicon substrate surface. The quantitative disagreement between the results of the present work and those of [7] for air can be explained by differences in experimental conditions.

The change in the components of the resulting heat transfer from the substrate holder to the substrate q_r, q_{tg}, q_{tdc} for hydrogen and argon filling the interlayer between them is presented in Fig. 3. We note that the main contribution to heat transfer in hydrogen is by conduction in the gas interlayer, whose value at atmospheric pressure is close to $0.80q_{res}$. The fraction of heat transfer by direct contact of the substrate with the substrate holder amounts to about $0.17q_{res}$, and that of radiation, $0.03q_{res}$. When the composition of the gas medium is changed (transition to argon), the relationship between these components (at atmospheric pressure) becomes: $q_{tg}:q_{tdc}:q_r$ = 0.25:0.64:0.11. A reduction of the pressure in the reaction chamber leads to an increase in the fraction of heat transfer by radiation, which compensates for the decrease in the fraction of heat transfer by conduction in the gas interlayer. Heat transfer by direct contact is independent of the pressure in the reaction chamber. Since $q_{tg} > q_{tdc}$, the heat flux direction deviates from the normal to the surface of contact between the substrate and its holder. This leads to the appearance of longitudinal (along the substrate) temperature gradient, which increases with a decrease in the value of q_{tg}, i.e., a decrease in the pressure in the reaction chamber. Under certain conditions [8], a longitudinal temperature gradient can result in thermoelastic stresses that cause crystallographic defects – so-called slip lines.

Figure 4 presents the results for the "underheating" of the substrate relative to the substrate holder θ as functions of the pressure in the reaction chamber, the gas flow rate, the gas medium composition, and the way in which the substrate is mounted on the substrate holder.

Let us consider the case when the gas flow rate through the reactor $V_g > 0$. At a pressure in the reactor corresponding to the regime of a continuous medium, the convective cooling of the substrate is increased with an increase in the gas flow rate (curve 3 and 4). A decrease in the gas flow rate displaces the point of inflection of the curves to the side of smaller pressures. An increase in the flow rate leads to linearization of the relations. When the substrate is separated from the holder by a distance of 3 mm, the flow rate and pressure have virtually no effect on the value of Θ in the range investigated. For comparison the figure presents the relation $\Theta = f(\bar{P})$ (curve 5) for hydrogen enclosed in a cylindrical tube with a wire heater located along the tube axis [8].

CONCLUSIONS

1. A decrease of the pressure in the reactor leads to an increase in the longitudinal temperature gradients, which cause crystallographic defects.

2. An increase of the ratio q_{tdc}/q_{tg} decreases the longitudinal temperature gradient.

NOTATION

d, diameter; $\bar{l}$, mean free path length of gas molecules; R, thermal resistance; T, temperature; ΔT, temperature difference; ΔT_j, temperature jump; q, specific heat flux; Kn, Knudsen number; α, heat transfer coefficient; Δ^*, thickness of gas interlayer between substrate and substrate holder; ε, emissivity; λ, thermal conductivity coefficient. Subscripts: g, gas; c, convection; r, radiant; o, atmospheric pressure; s, substrate; wp, working pressure; w, wall of reaction chamber; 1, "substrate holder–substrate" system; 2, "substrate–reaction chamber wall" system; sh, substrate holder; red, reduced; dc, direct contact; res, resultant; tdc, thermal conductivity of direct contact; tg, thermal conductivity of gas interlayer.

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