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The effect of the rate of temperature change on the thermomigration of liquid inclusions in silicon

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Abstract. The influence of the rate of temperature change of the composition on the consistency of the processes of dissolution, crystallization and atomic transfer in a liquid inclusion and at its boundaries, characteristic of stationary conditions of thermomigration, is theoretically estimated. Using the example of the silicon-aluminum system, the effect of stepwise and smooth temperature changes on the processes determining thermal migration and the velocity of movement of the liquid inclusion is established. A critical rate of temperature change has been found, above which thermomigration becomes impossible.

Keywords: thermomigration, silicon, crystallization, dissolution

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Материалы конференции

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Влияние скорости изменения температуры на термомиграцию жидких включений в кремнии

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Аннотация. Теоретически оценено влияние скорости изменения температуры композиции на характерную для стационарных условий термомиграции согласованность процессов растворения, кристаллизации и атомарного переноса в жидком включении и на его границах. На примере системы кремний-алюминий установлено влияние ступенчатого и плавного изменения температуры на процессы, определяющие термомиграцию и скорость движения жидкого включения. Найдена критическая скорость изменения температуры, выше которой термомиграция становится невозможной.

Ключевые слова: термомиграция, кремний, скорость нагрева, скорость охлаждения, скорость миграции

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Introduction

Thermomigration (TM) of liquid inclusions (zones) in solids under the action of a temperature gradient is used in physico-chemical studies and for the formation of electrically heterogeneous structures in a silicon wafer [1–4]. The movement of the zones is caused by the recrystallization of silicon through a metal-based solvent zone, which lowers the temperature of formation of the liquid phase. The rate of TM under stationary conditions is determined by three self-consistent processes: dissolution at the “hot” boundary of the zone, diffusion transfer of atoms through the zone and crystallization at the “cold” boundary. The advantage of the TM method is the high recrystallization rate, which is 3–4 orders of magnitude higher than the rate of solid-state diffusion. This makes it possible to form channels not only on the surface, but also in the volume of the wafer.

In stationary TM conditions, the temperature of the zone increases as it migrates in the direction of the temperature gradient and usually does not exceed several degrees. This ensures quasi-isothermal conditions of the process, which is important for the uniformity and crystal perfection of the formed structures. The temperature of the zone can be changed by regulating the power of the heating device, which inevitably occurs when the composition is heated before entering stationary mode and when cooled after TM. Moreover, the heating or cooling time is commensurate with the time of the stationary mode. In particular, the temperature change causing supersaturation or undersaturation of the melt solution is an additional driving force for the crystallization and dissolution processes at TM, which has not been studied. The effects of abrupt (stepwise) and smooth (slow) temperature changes on the processes occurring in the zone are different. Previously, the influence of only small temperature fluctuations in the TM process was considered in the literature [5]. The rate of temperature change can affect the interrelated processes of dissolution, crystallization and atomic transfer in the zone, which determine the velocity and shape of the liquid zone. The aim of the work is theoretically assess this effect using the example of the silicon-aluminum system.

Stepwise temperature change

The temperature T in the zone is established much faster than the concentration of components in the melt solution, since the coefficients of thermal conductivity and diffusion differ by about three orders of magnitude. Therefore, with a stepwise temperature change, the establishment of the concentration distribution necessary for TM in the zone is delayed for some time.

Let's estimate the value of τ using a one—dimensional numerical model of mass transfer based on the diffusion equation

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2},$$

where $D(T)$ and $C(x,t)$ are the diffusion coefficient and the silicon concentration in the zone, t is current time, x is coordinate in the direction of the temperature gradient G (Fig. 1, *a*).

The initial distribution of the concentration $C(x, 0)$ corresponding to the stationary regime of TM is shown on curve 1 (Fig. 1, *b*), which shows the temperature differences at the boundaries of the zone necessary for the continuous processes of dissolution and crystallization. A stepwise change in temperature causes a change in the concentration of silicon at both boundaries of the zone according to the phase diagram of the system. In this case, the thickness of the zone increases or decreases proportionally if the temperature jump is positive or negative. The time of equilibrium of concentration at the boundaries of the zone is neglected, since the temperature

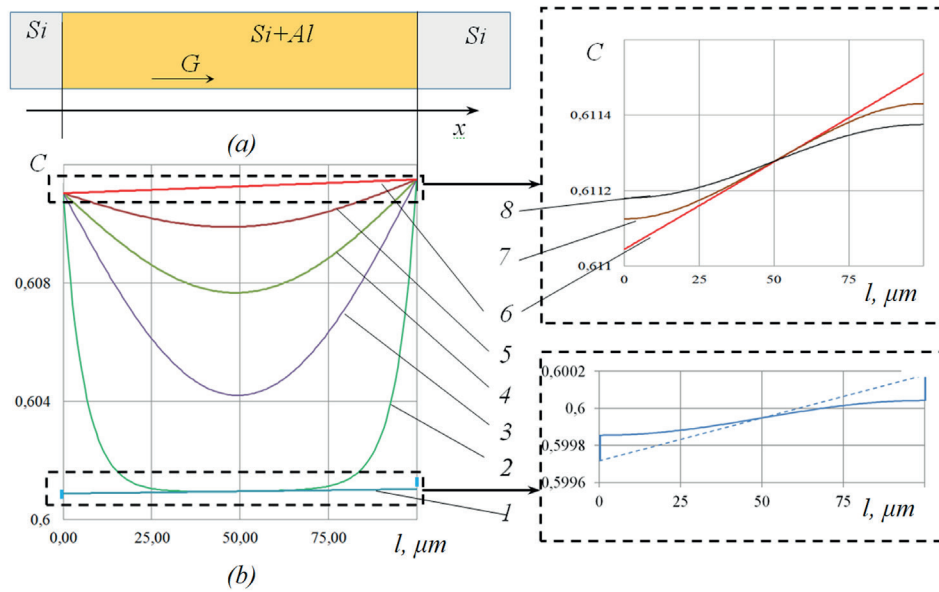


Fig. 1. Diagram of the liquid zone motion model (a) and the distribution of silicon concentration in the liquid phase at $t = 0; 0.003; 0.06; 0.12; 0.21; 0.9; 0.95; 1$ s (curves 1 – 8) (b)

jump is greater than the temperature drop in the zone. Fig. 1, b shows as an example the calculated curves (2 – 8) of the distribution of silicon concentration in the zone for different time points at an initial temperature $T = 1373$ K, $G = 40$ K/cm, $l = 100$ microns for a temperature jump of 10 K. Upon reaching the concentration distribution (curve 6, Fig. 1, b) in the boundary conditions of the diffusion problem, deviations of concentration from equilibrium values were taken into account, which is necessary for the implementation of atomic kinetic processes at both boundaries of the zone (Fig. 1, b).

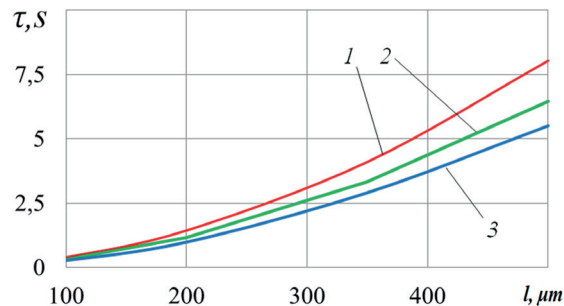


Fig. 2. Dependence of the time of establishment of the stationary regime on the thickness of the flat zone at different values of the TM temperature
1 – $T = 1173$ K, 2 – $T = 1373$ K, 3 – $T = 1573$ K

During the simulation, it was assumed that the concentration differences in the zone necessary for the coordinated processes of crystallization, dissolution and diffusion have the same values. The variation of these differences had a slight (within 5%) effect on the time of establishing a stationary concentration distribution. The total setting time was 0.5 – 8 s for typical TM conditions. The value of τ depended most sharply on l , less sharply on T (Fig. 2) and practically did not depend on the value of temperature jump. During this period of time, the zone stopped, and then continued to migrate at a constant rate corresponding to the new temperature value.

Smooth temperature change

Such a temperature change affects the atomic kinetic processes of dissolution or crystallization and causes inhibition or blocking of boundary movement. An increase in temperature inhibits

crystallization at the “cold” boundary of the zone and promotes dissolution at the “hot” one. Lowering the temperature makes it difficult or blocks dissolution at the “hot” boundary and promotes crystallization at the “cold” one. Blocking any of these processes stops the movement of the zone.

We find the critical velocity of the acr blocking the movement of the zone, based on the thicknesses of the layers grown (or dissolved) due to thermal migration of h_G and cooling (or heating) h_T at one of the boundaries of the zone in a short period of time Δt : $h_G = v \Delta t$ and $h_T = 0.5 \Delta C l$. Here v – speed of movement of the zone, ΔC – change in silicon concentration with a temperature change by ΔT during Δt : $\Delta C = \frac{dC}{dT} \Delta T$, where dC/dT – cotangent of the angle of inclination of the liquidus line of the system state diagram, $\Delta T = a_{cr} \Delta t$. The change in the volume of silicon during the phase transition is small and it is not taken into account. Equating h_G and h_T , we obtain the formula for the critical rate of temperature change $a_{cr} = 2v/l$. The numerical value of a_{cr} for typical TM conditions was 1 – 10 K/s (Fig. 3).

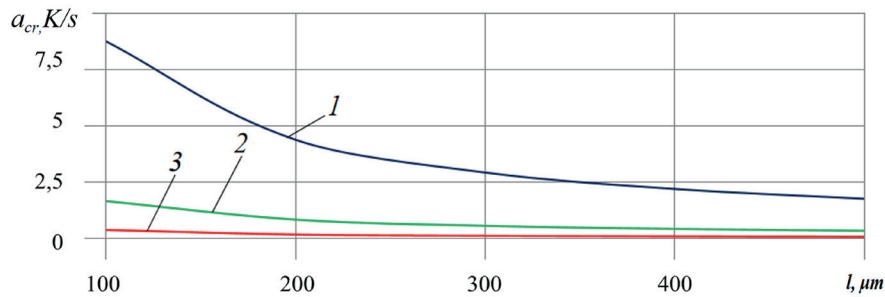


Fig. 3. Dependence of the critical rate of temperature change on the thickness of the flat zone at different temperature values
 1 – $T = 1173$ K, 2 – $T = 1373$ K, 3 – $T = 1573$ K

If the actual rate of temperature change is greater than the critical one, then the movement of the zone is impossible due to the blocking of one of the two processes at the boundary of the zone, depending on the heating or cooling of the composition. At $a < a_{cr}$, the velocity of movement of the zone can both decrease and increase. The decrease v corresponds to the same difficulty of crystallization and dissolution processes. However, dissolution is more difficult for the Si-Al system [1], which leads to deformation (compression) of the zone in the direction of movement. By adjusting the heating rate during the TM process, it is possible to relax the restrictions at the dissolution boundary, while maintaining an acceptable crystallization rate. In this case, an increase in the velocity and a decrease in the degree of deformation of the zone is achievable.

Conclusion

A stepwise change in the temperature of the composition at TM stops the movement of the zone for a short time, and with a smooth change in temperature, the velocity of the zone can both decrease and increase at heating or cooling speeds lower than the found critical value. When the temperature change rates exceed the critical one, the movement of the zone becomes impossible. In the area of speeds lower than the critical one, temperature changes in the TM process can control the deformation of the zone.



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