Transformation of the circular zone during thermal migration in silicon in the direction $\langle 100\rangle$

© B.M. Seredin, V.P. Popov, A.V. Malibashev, A.D. Stepchenko

Platov South-Russian State Polytechnic University (NPI), 346428 Novocherkassk, Russia E-mail: seredinboris@gmail.com

Received April 26, 2024 Revised July 20, 2024 Accepted October 30, 2024.

Aluminum-based circular zones make it possible to form a system of through-closed epitaxial channels of *p*-type conductivity in a silicon wafer without crossing adjacent zones, which eliminates the possibility of zone rupture characteristic of intersecting linear zones and increases the reproducibility of the thermomigration method. The peculiarities of the transformation of ring zones at various stages of migration in silicon in the direction $\langle 100 \rangle$ have been experimentally revealed. The observed changes in the shape of the zones and epitaxial channels are due to the asymmetry of the dissolution front of the liquid zone caused by the features of the cut caused by the bending of the linear zone. At the same time, the cutting of the singular planes of the inner contour of the zone is suppressed and preserved on the outer one.

Keywords: Thermomigration, temperature gradient, silicon.

DOI: 10.61011/SC.2024.09.59916.6414A

1. Introduction

Thermomigration (TM) of liquid zones in solids under the action of a temperature gradient has long been known as a method for creating electrically heterogeneous structures in the bulk of a crystal [1,2]. The processes and phenomena that define and accompany TM are still actively studied [3,4]. Attempts to implement TM in power electronics [5] confirmed the unique capabilities of the method for forming a system of end-to-end epitaxial uniformly doped channels in silicon wafers in the form of closed cells. In this case, closed square cells of the *p*-type of conductivity were obtained using an orthogonal grid of rectilinear aluminum-based zones migrating through a silicon wafer. However, the resulting discontinuities of linear zones near their intersections did not ensure the preservation of the specified cell topology and the TM reproducibility necessary for industrial production.

It is known that maintaining a given topology of a system of rectilinear zones requires a uniform temperature gradient field perpendicular to the wafer and the fulfillment of certain orientation conditions that take into account the anisotropy of a crystal [2,6]. According to the specified conditions, the grid of orthogonal linear zones on the starting surface of the wafer should have directions $\langle 110 \rangle$.

The trajectory of the rectilinear zone may not coincide with the direction of the temperature gradient. Such a deviation is observed if the faceting results in an asymmetrical shape of the dissolution front relative to the temperature gradient [2]. The TM force model [7] allows estimating the value of the angle of deviation of the trajectory of the zone from the normal. According to the model, the forces of resistance to atomic kinetic dissolution processes in individual sections of the dissolution front are proportional to the areas of the sections and perpendicular to them. The deviation of the vector sum of these forces from the direction of the temperature gradient leads to a tangential displacement of the zone. The use of isolated closed linear zones in the shape of a square in case of TM allows avoiding intersections and contributing to the reproducibility of the TM method [8]. The purpose of this paper is to experimentally study the transformation stages of the annular zone during its migration in silicon in the $\langle 100 \rangle$ direction and explain the asymmetry of the zone cross-section that causes the transformation.

2. Experiment

Annular zones with a diameter of 1 to 5mm were created on the starting surface of a silicon wafer by magnetron deposition of an aluminum layer with a thickness of $10\,\mu\text{m}$, followed by projection photolithography. Single crystal wafers *n*-type, resistivity $4.5 \Omega \cdot cm$, orientation $(100) \pm 0.5^{\circ}$ with a diameter of 100 mm and a thickness of 0.5 and 0.8 mm with a dislocation density of $10^2 \, \text{cm}^{-2}$ were used. The width of the aluminum rings was $100 \,\mu$ m. TM was carried out in a vacuum water-cooled chamber at temperatures 1270-1570 K and temperature gradients 20-100 K/cm for 20-240 min. A specially designed heating device [9] provided a uniform temperature gradient field in the silicon wafer (tangential component of the temperature gradient < 1 K/cm). The shape of the zones and channels was studied metallographically on planar and transverse polished surfaces of the wafers.

It was found that the annular zone changes its shape during migration and turns into a square with corners elongated in the direction of $\langle 100 \rangle$ (Figure 1). The trans-

451



Figure 1. Photographs of the epitaxial channel obtained at a TM temperature of 1400 K using an annular zone in case of TM at various distances from the starting surface, μ m: 10 (*a*), 170 (*b*), 750 (*c*). The outer diameter of the annular zone is 2.2 mm.



Figure 2. Photograph of a cross-section of a closed cell formed by an annular zone. The cross section is in the direction of $\langle 110 \rangle$ along the diameter of the zone. The finish surface of the wafer is at the bottom. TM process temperature is 1300 K.



Figure 3. Photograph of an epitaxial channel obtained at a TM temperature of 1450 K using an annular zone with segments of rectilinear zones at various distances from the launch surface, μ m: 50 (*a*) and 510 (*b*).

formation of the annular zone begins with the appearance of facets at four points located symmetrically on the outer contour of the annular zone (marked with arrows in Figure 1, a). Rectilinear sections of the zone appear along the directions $\langle 110 \rangle$ in these points, migrating into the interior of the zone at an angle $\alpha < 35^{\circ}$ relative to the normal to the wafer (Figure 1, b). There is no cut on the inner contour of the zone. The lengths of these sections monotonously increase until the formation of a zone in the form of a square (Figure 1, c). The sides of the square converge at the same angles α as the faceted sections of the annular zone. The angle α decreased from 33 to 15° with an increase of the process temperature from 1270 to 1570 K. As a result, a continuous closed cell of a complex pyramidal shape is formed. The ring zone system migrated through the wafer without compromising its integrity in the studied conditions and size ranges.

A feature of the transformation of the annular zone near $(60-100\,\mu\text{m})$ the finishing surface of the wafer is revealed: the inclined trajectories of the approaching sections of the zone become normal ($\alpha = 0^{\circ}$) surfaces (Figure 2). This effect always appears and does not depend on at what stage of transformation the zone reaches the finish surface.

An attempt has been made to eliminate the transformation of the annular zone into a square one by setting four radial segments of zones on the starting surface of the wafer at the points of cut origin (Figure 3). The segments of the zones were oriented in the directions $\langle 110 \rangle$. It can be seen that the zones with such segments retained their original ring shape. However, breaks occurred at the junctions of the rectilinear segments of the zones to the annular zone. Studies have shown that they are initiated by the appearance of protrusions on the inner contour of the annular zone opposite the segments on the outer contour in the plane of the wafer. The development of these protrusions in the tangential direction led to the observed discontinuities of the zone.

3. Results and discussion

The explanation of the transformation of the annular zone in TM is related to the peculiarities of the asymmetry of the shape of the dissolution front caused by faceting in certain areas of the annular zone (Figure 1). The presence of a faceted dissolution or crystallization front indicates a layered mechanism of processes at the interphase boundary, which requires a greater driving force than at the atomic-rough boundary. The faceting of the interphase front does not occur if there is a source of atomic steps on a singular surface. The concave front of the dissolution zone excludes the presence of natural atomic steps and is bordered by singular planes {111}.

The zone transformation begins at four points on the annular zone, the tangents to which coincide with the directions $\langle 110 \rangle$, where the planes of faceting originate on the outer contour of the zone dissolution. A symmetrical

cutting plane characteristic of the rectilinear zone does not occur on the inner contour, due to the negative curvature of the inner contour of the zone, which has atomic steps that facilitate the dissolution of the crystal. Therefore, a lateral force of resistance to movement appears at these four points, directed inside the annular zone and leading to the formation of a square-shaped zone. The observed effect of the convergence of the sides of the square zone during further TM is determined by the peculiarities of the dissolution and crystallization process in the corners of the squares. The angle on the outer contour of the zone makes it difficult to dissolve, and the angle on the inner contour, due to the negative curvature, provides atomic steps that facilitate dissolution. Atomic steps in the corner on the inner contour of the zone extend along the boundary and prevent the formation of cutting planes on adjacent rectilinear sections of the inner contour, while maintaining the cutting plane on the outer contour. An asymmetric facet appears on the dissolution front, explaining the synchronous convergence of the sides of the square.

The detected change in the trajectory of the rectilinear sections of the initially annular zone near the finish surface is associated with the atomic roughness of the wafer surface. As soon as the liquid zone touches the finish surface, atomic steps spread from the surface along the plane of the facet on the outer contour and suppress it. The liquid zone then moves in the direction of the temperature gradient across the wafer.

The use of straight line zone segments at four characteristic points of the ring zone stopped the development of the zone transformation. The discontinuities of the annular zone with radial segments are explained by the difference in conditions on the inner and outer contours of the zone at the junctions of the segments to the annular zone. Two corners are formed on the outer contour of the zone, which are the sources of atomic steps. This creates an additional driving force due to the gradient of the chemical potential, leading to the transfer of silicon in the liquid zone in the tangential direction. A protrusion appears on the inner contour, and a dissolution area appears on the outer contour. The development of these processes leads to the TM result observed in Figure 3.

4. Conclusion

It was found that the annular zone under thermal migration in silicon in the direction of $\langle 100 \rangle$ changes its shape and turns into a square, followed by synchronous convergence of opposite sides with the formation of elongated angles in the directions of $\langle 100 \rangle$ in the plane of the wafer. The convergence of the sides stops near the finish surface, and the trajectory of the zones becomes a normal surface. The observed effects are explained by the peculiarities of silicon dissolution on the inner and outer contours during bending of the linear zone in the wafer plane. It was found that rectilinear segments of zones adjacent to the outside of the annular zone at the points of cut origin prevent the transformation of the annular zone into a square one and can lead to breaks in the annular zone at the junctions during migration.

Funding

The work was carried out with the support of the Ministry of Science and Higher Education of Russia as part of the state assignment to the Platov South Russian State Polytechnic University (NPI) on the topic FENN-2023-0005.

Conflict of interest

The authors declare that they have no conflict of interest.

References

- [1] W.G. Pfann. Zone Melting (Wiley, N.Y., 1963).
- [2] V.N. Lozovsky, L.S. Lunin, V.P. Popov. Zonnaya perekristallizatsiya gradientom temperatury poluprovodnikovykh materialov (Moscow, Metallurgy, 1987). (in Russian).
- [3] S. Pawar, K.P. Wang, A. Yeckel, J.J. Derby. Acta Mater., 228, 117780 (2022). https://doi.org/10.1016/j.actamat.2022.117780
- [4] S.I. Garmashov. J. Cryst. Growth, 627, 127532 (2024). https://doi.org/10.1016/j.jcrysgro.2023.127532
- [5] O.S. Polukhin, V.V. Kravchina. Technol. Design Electron. Equipment, 1–2, 34 (2023). http://dx.doi.org/10.15222/TKEA2023.1-2.34
- [6] T.R. Anthony, J.K. Boah, M.F. Chang, H.E. Cline. IEEE Trans. Electron Dev., 23 (8), 818 (1976).
 DOI: 10.1109/T-ED.1976.18492
- B.M. Seredin, V.P. Popov, A.V. Malibashev, I.V. Gavrus, S.M. Loganchuk, S.Y. Martyushov. Silicon, 16, 3453 (2024). DOI: 10.1007/s12633-024-02921-0
- [8] B.M. Seredin, V.P. Popov, A.V. Malibashev. Pis'ma ZhTF, 50 (7), 17 (2024). (in Russian).
 DOI: 10.61011/PJTF.2024.07.57463.19805
- [9] B.M. Seredin, V.P. Popov, A.V. Malibashev, I.V. Gavrus, A.A. Skidanov. RF Patent 2805459 (2023). (in Russian).

Translated by A.Akhtyamov