ISSN: 0975-8585

Research Journal of Pharmaceutical, Biological and Chemical Sciences

Electromigration Processes in Silicon Single Crystals Involving Melt Inclusions.

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ABSTRACT

We studied formation and dynamics of melt inclusions in silicon single crystals at direct and pulse current flowing. It is ascertained that a general regularity of migration of impurity regions in Si is simultaneous precipitation of matrix atoms from a melt drop and their dissolution in it under the action of both Peltier heat localized at interphase boundaries and the electromigration forces in the inclusion bulk. It is found experimentally that dimensional dependence of inclusion migration velocity obeys a linear law at flowing of direct currents ($j<5\cdot10^6$ A/m^2) as well as rectangular current pulses ($j<10^7$ A/m^2, 100 μs<τ<1000 μs). The contributions from electromigration and Peltier heat to the resulting velocity of migration of impurity regions by electric current are determined. The contribution from electromigration decreases as inclusion thickness increases, the other conditions being the same.
Keywords: silicon single crystals, melt inclusions, semiconductors, migration velocity, silicon

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ISSN: 0975-8585

INTRODUCTION

Formation and dynamics of impurities in semiconductors as melt regions occur, as a rule, when the critical operating conditions for power semiconductor devices (transistors, Peltier elements, etc.) are reached [1-3]. In this case, as is known [4,5], the near-contact regions and metal–semiconductor contacts may heat up to temperatures over the melting points for eutectics of relatively fusible systems (Al-Si, Ag-Si, Au-Si; the melting point for Au-Si eutectic T_e = 370°C).

To illustrate, during operation of a thermoelectric generator for automobile internal-combustion engines developed in [6], certain modules or their parts may be heated for a short time to temperatures over 330°C. The result can be fusion of structure fragments and their failure. And this happens despite equalizing of temperature field (provided with the construction of heat-exchange apparatus) at the hot side of thermoelectric modules [6]. Obviously failure of electric contact in a thermoelectric module because of overheating will lead to failure of the whole system, thus considerably reducing the efficiency of thermoelectric generator.

During operation of such devices, a direct electric current consumed by the resistive load is flowing through each module. At overheating and beginning of fusion, the current flows through the liquid phase–crystal contact. This makes it necessary to study the electromigration processes at the semiconductor surface and in the bulk involving melt regions that are proceeding under the action of direct and pulse currents.

In those cases, migration of the produced liquid phase in electric field is possible in the system studied. The field of crystal structural non-uniformity (gradient of dislocation density) also can promote migration of the melt regions [7,8]. These are just the above factors that cause the interest of researchers in the electromigration processes at the semiconductor surface and in the bulk involving melt regions [9].

As a rule, migration of liquid inclusions in semiconductors is related to transfer of matrix atoms from one inclusion boundary to another through the inclusion itself. An inclusion migrates because the matrix atoms are dissolving at the forward inclusion wall, then they are diffusing through the inclusion and at last become deposited onto the matrix at the back wall, with formation of new atomic layers. In the case of liquid inclusions, solubility of matrix atoms in the inclusion and the coefficient of diffusion of these atoms in the inclusion bulk are sufficiently high, so such a migration mechanism is crucial [10,11].

With such a mechanism, flowing of electric current through the liquid phase–crystal contact is accompanied by Peltier heat release at the one interphase boundary and absorption at the other interphase boundary: $\pm Q_P = Pjt$. (Here P is the Peltier coefficient at the melt–crystal interface, j is the current density, t is the time of current action.) This leads to variation of concentrations at the inclusion walls and requires accounting for thermoelectric effects in the course of mass transfer. Besides, one should also take into account the effect of electromigration that creates concentration non-uniformity near the interphase boundaries, depending on the value and sign of the effective charge Z^* of semiconductor atoms in the melt [10,11].

When determining the predominant role of the above mechanisms, one should note that for inclusions of sizes

$$\ell >> \sqrt{\frac{D\tau}{\pi}} \qquad (1)$$

(τ is the current pulse duration), only the contribution from Peltier heat is significant at migration. A qualitative experimental confirmation of this statement was made for elementary semiconductors of *p*- and *n*-type. At pulse duration τ = 150 μs and pulse height I = 6·10^3 A, migration of drops of the Al, Ga, Ag melt occurred towards anode and was determined by the thermoelectric effects at the interphase boundaries. In the stationary regime, inversion of drop velocity was observed (the drops moved towards the negative electrode). This indicated the predominant role of electromigration. Unfortunately, application of nonstationary heating of semiconductor and surface migration only prevented obtaining dimensional dependence of migration velocity.

Therefore, the aim of the present work was investigation of dimensional dependence of migration velocity for melt Al-Si inclusions in silicon under direct and pulse electric current action.

MATERIALS AND METHODS

The experiments were performed in a vacuum chamber for silicon (*n*-type, resistivity of 10 Ω·cm) specimens that were previously cut into 4×4×15 mm blocks. After lapping with M-15 micropowder and with ACM-5 diamond paste, the specimens were treated with ethanol and then were clamped between two tantalum electrodes by the procedure described in [10,11] in a quartz electric resistance furnace. 5 mm thick graphite spacers were put between the specimen and electrodes to prevent their contact interaction. The electrodes were connected to the dc source through an ammeter using copper wires. When performing experiments with current pulses, we used a rectangular pulse generator. The pulse duration and height were τ = 100–1000 μs and I = 5–30 A respectively.

Before performing the experiment, the chamber was vacuumized down to a residual pressure of ~50 Pa. Then it was filled with argon up to a low excess pressure. In the course of experiment performance, the electrodes and the whole working chamber were cooled with water from the water cooling board.

At migration in the bulk, an aluminum plate (mass of 0.6–0.9 mg) was put between the {111} planes of two specimens. Then they were heated up to a temperature close to the experiment one (T = 1000–1123 K). The experiment temperature was determined by the net effect from the space heater and electric current flowing through the specimen*.

In the course of experiment performance, the temperature of the specimen was determined either using the thermocouple method or from the specimen luminosity. In the latter case, the temperature regimes in the experiments were registered with a pregraduated photocell located on one of the eyepieces of a high temperature microscope. The temperature measurement error was no more than ±10%. The distribution of temperature T and concentration C of semiconductor atoms (dissolved in inclusion) during migration of the melt region are presented in Fig. 1.

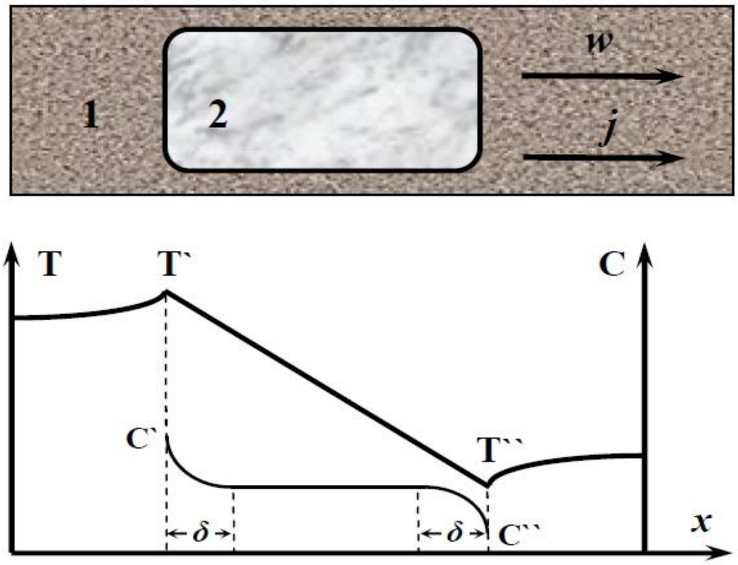

Figure 1: Schematic of migration of melt region: 1 - semiconductor matrix; 2 - melt inclusion. Distribution of temperature *T* and concentration *C* of semiconductor atoms (dissolved in inclusion) during migration of the melt region.

RESULTS AND DISCUSSION

An occurrence of melt regions in the silicon matrix bulk at stationary electric annealing is related to formation of an alloy between an Al film and Si single crystal. This mechanism obeys the reaction-diffusion law: a new phase is formed that was not found before interaction between components. Its growing is given by the following expression:

$$x = 2\beta\sqrt{D\tau_k}\ . \qquad (2)$$

Here D is the reaction-diffusion coefficient; β is an argument of the Kramp function that is determined from the diagram of phase equilibrium. Thereby a melt film is formed at the metal–semiconductor interface as the proper temperature is reached. Thermodynamic instability of the film promotes its dispersion into drops. The inclusions generated in such a way drift in an electric field.

An analysis of numerous experimental data obtained for the Al-Si system showed that, in the course of migration, melt inclusions are faceted by specific crystallographic planes that shape inclusions into a distinguishing feature (Fig. 2). In this case, the electric current flowing through the inclusion does not distort the form of drifting regions.

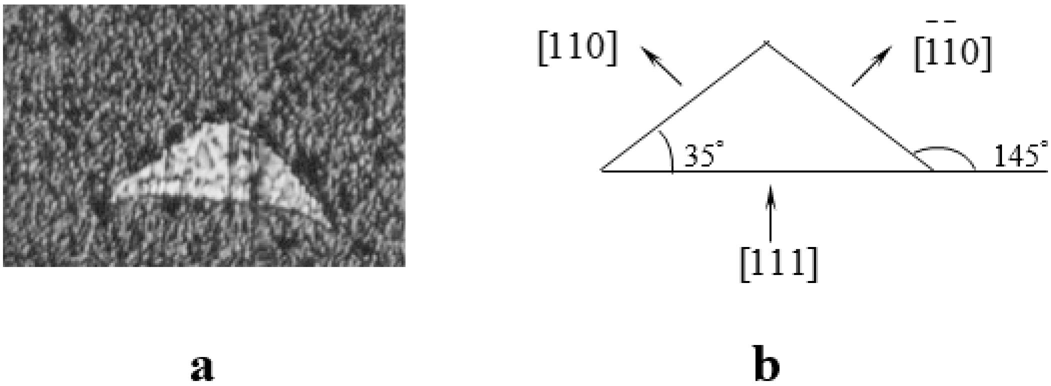

Figure 2: A pattern of Al-Si inclusion in single crystalline silicon. The section plane: ⊥(111). Magnification: ×200.

To determine crystallographic indices of the faceting planes at migration of the Al-Si system, the equation of structural crystallography for a cubic lattice [12] was used:

$$\cos\varphi = \frac{h_1h_2 + k_1k_2 + l_1l_2}{\sqrt{h_1^2 + k_1^2 + l_1^2} + \sqrt{h_2^2 + k_2^2 + l_2^2}}\ . \qquad (3)$$

Here φ is the angle between the planes; h_i, k_i and l_i are the indices of crystallographic planes. According to the experimental data, an angle φ between the {111} plane and those with unknown indices {h_2, k_2, l_2} is 35 or 145 deg for which cosφ = +0.819. A good agreement between the experimental and theoretical values of cosφ can be obtained if (110) and ($\bar{1}\bar{1}0$) will correspond to the indices h_2, k_2 и l_2: substitution of the above values in Eq. (3) gives cosφ = +0.821.

The inclusion size ℓ and depth of inclusion penetration in the matrix from the starting position were determined by sequential removal of N layers (at every 5–10 μm) [10,11,13] with subsequent identification of inclusions using a microscope МИИ-4.

The typical results of investigations are presented in Fig. 3. As before [10,11,14], the dimensional dependence of migration velocity is linear. To identify the origin of driving forces that determine inclusion migration in electric field in the case of predominance of transfer processes in inclusion bulk, let us use the equation from [10]:

$$\frac{w}{j} = -\frac{VD\overline{C}}{N_A}\left(\frac{\rho e Z^*}{kT} + \frac{VP\,L}{\delta N_A 2\lambda kT^2}\cdot \ell\right) \qquad (4)$$

That takes into account the contributions from electromigration and Peltier heat at flowing direct electric current of density *j*. Here *w* is the velocity of inclusion migration; *V* is the melt specific volume; $\overline{C}$ (*D*) is the equilibrium concentration (diffusion coefficient) of semiconductor atoms in the melt; N_A is the Avogadro's number; δ is the thickness of diffusion layer at the interphase boundary; ρ is the melt resistivity; *e* is the elementary charge; *k* is the Boltzmann constant; *L* is the heat of transition of unit volume of solid phase into the melt; λ is the melt coefficient of thermal conductivity evaluated using the Wiedemann–Franz law. For a stationary electric annealing (1, Fig. 3), Eq. (4) agrees fully with experiment if *P* is considered negative and Z^* is considered positive.

At pulse current action, the character of dimensional dependence is changed - see 2 and 3, Fig. 3. Reduction of pulse duration leads to increase of velocity for inclusions of the same size. We relate the main responsibility for the observed variations to reduction of the contribution from electromigration.

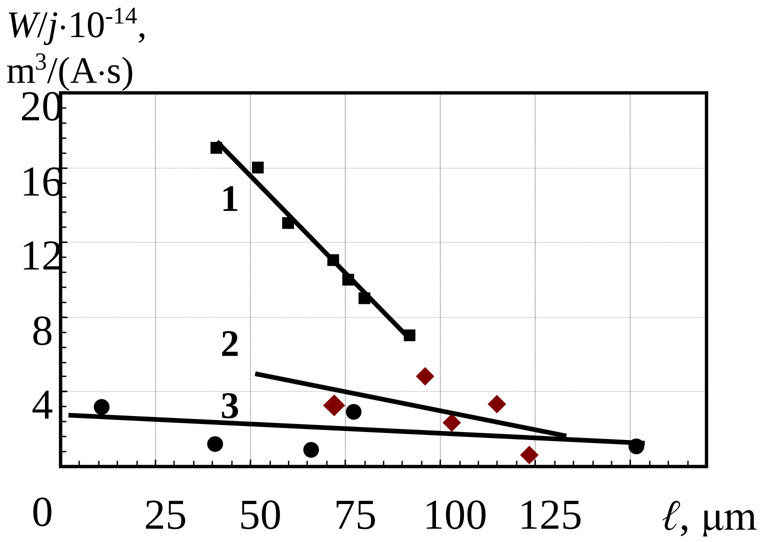

Figure 3: Dimensional dependence of migration of Al-Si inclusions in the bulk of single crystalline silicon at *T* = 1073 K at flowing: 1 - direct current of 12 A; 2 - rectangular current pulses of height I_{max} = 24 A and duration τ = 300 μs; 3 - I_{max} = 24 A and τ = 900 μs.

Indeed, at *P*<0 the concentration non-uniformity at interphase boundaries is provided by heat release (absorption) Q_P at the cathode (anode) interphase boundary. This promotes inclusion migration because of melting–crystallization at the interphase boundaries along the electric field lines (just as observed in the experiment). Electromigration (Z^*>0) will produce the opposite gradient, thus reducing $\partial C / \partial x$ of the thermoelectric origin.

CONCLUSION

So migration of inclusions at stationary electric annealing of Si crystals is determined by heat release at the interphase boundaries that ensures migration of inclusions towards the negative electrode. Electromigration produces the opposite gradient which decreases the resulting inclusion velocity. The smaller the length of electric current pulses is, the weaker is their effect on reduction of the contribution from electromigration to the resulting inclusion velocity. This shows itself most clearly at pulse duration τ = 300 μs.

ACKNOWLEDGEMENT

This paper was prepared within the Agreement # 14.577.21.0078 dated June 5, 2014 for a subvention funded by the Ministry of Education and Science of the Russian Federation. Unique identifier for Applied Scientific Research RFMEFI57714X0078.

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