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# Influence of the growth regime on the transport properties of doped $Mg_2Si$ films

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**Abstract.** In this work, we studied transport properties of the doped $Mg_2Si$ film on silicon substrate. The ~1 μm-thickness film was synthesized by the solid phase epitaxy method. Well-proven Ag was chosen as a dopant. At room temperature, the resistivity was 2 Ω×cm, the mobility was 327 $cm^2/(V×s)$, the density was $9.3×10^{15}$ $cm^{-3}$. We established that using the solid phase epitaxy with the low temperature annealing regime led to mixed electron conductivity of the doped $Mg_2Si$:Ag film due to the substitution of Si-site by Ag. The activation energy of the donor level is 24 meV.

**Keywords:** silicon, magnesium silicide, solid phase epitaxy, silver, Hall-measurements, SEM, EDX

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# Влияние режима роста на транспортные свойства легированных плёнок $Mg_2Si$

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**Аннотация.** В работе исследованы транспортные свойства легированной пленки $Mg_2Si$ на кремниевой подложке. Пленка была сформирована в условиях сверхвысокого вакуума методом твердофазной эпитаксии, ее толщина составляет ~1 мкм. В качестве легирующей примеси было выбрано хорошо зарекомендовавшее себя серебро. Подвижность носителей заряда составила 327 $см^2/(В \times с)$, концентрация носителей — $9.3 \times 10^{15}$ $см^{-3}$.

**Ключевые слова:** кремний, силицид магния, твердофазная эпитаксия, серебро, холловские измерения, СЭМ, ЭДС

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## Introduction

Recently, thin-film thermoelectric converters (TEC) have attracted the attention of researchers due to their wide range applications. They could be used as power sources for microwatt devices [1], heat flow sensors [2], and coolers for local thermal management [3]. Also, thin-film TEC could be combined with photovoltaic and thermophotovoltaic cells in hybrid converters [4]. The most popular thermoelectric compounds include expensive and toxic chemical elements that limits their wide commercial distribution. Silicide-based thermoelectric converters are considered as feasible low-cost and eco-friendly alternative. Among them, $Mg_2Si$-based materials demonstrate competitive properties [5]. The bulk samples are well-researched but there is a lack of works on synthesis and transport measurements of doped films.

## Materials and methods

Substrates were cut from floated zone silicon with >1000 Ω×cm resistivity and (111) orientation. First, silicon substrates were washed by isopropanol, and then rinsed in Piranha solution and deionized water. After loading cleaned samples in ultra-high vacuum chamber series of degassing cleaning was conducted at 600 °C and 850 °C for 12 hours and 20 minutes, respectively, for the $SiO_x$ removing. $Mg_2Si$ films were synthesized by solid phase epitaxy (SPE) at ultra-high vacuum condition (~$10^{-9}$ Torr). Amorphous Mg-Ag mixture was deposited on the cleaned Si surface at room temperature. Then, we conducted recrystallization annealing at 300, 330 and 360 °C consequently without interrupting molecular flows. The $Mg_2Si$ forming was proofed by infra-red Fourier spectroscopy. For Hall measurements, metallic pads (Ti-Au) were deposited and annealed in argon atmosphere at 450 °C for 20 minutes to create ohmic contacts. Hall-measurements were carried out in Van der Pauw geometry. The film thickness was estimated by scanning electron microscopy. Stoichiometric ratio was established by X-ray energy dispersive spectroscopy.

## Results and discussions

As a result of these growth procedures, a 1 μm-thickness film was synthesized with Mg:Si = 2:1 stoichiometric ratio. Carrier density at room temperature was $9.3 \times 10^{15}$ $cm^{-3}$, mobility was 327 $cm^2/(V \times s)$ and resistivity was 2 Ω×cm. The characteristic feature of the film synthesized by the described method is electron conductivity with moderate doping level. Previously, in many papers, the Ag impurity was used as an acceptor [6, 7]. This phenomena could be caused by the following. Theoretical works say that Ag impurity can be both donor and acceptor depending

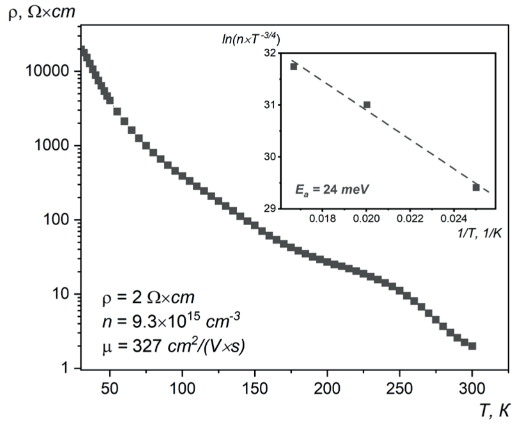


Fig. 1. Temperature dependence of the resistivity from 30 to 300K, main transport coefficients at the room temperature and activation energy of Ag-donor impurities in the insert

on the occupied site [8]. An acceptor level is formed when an Ag atom substitutes a Mg-site. This scenario has the highest probability. A donor level is caused by occupation of a Si-site or a 4b-site by an Ag atom. It should be noted that probability of these scenarios was estimated at 1105 °C that is much more than experimental temperature regime. Also, in reported works, the doping was conducted after the crystallization of $Mg_2Si$ at high temperature (450–500 °C) [6, 7]. This temperature could lead to desorption of Mg atoms that produced vacancy occupied by Ag impurity. In our case, the Mg-Ag mixture was firstly deposited on the Si surface. So, due to the increased diffusion length there is some Si deficit in the $Mg_2Si$ film. The occupation of these Si vacancies by Ag atoms led to the donor level formation [8].

## Conclusion

In this work, we reported about the Ag-doped $Mg_2Si$ film growth on the silicon substrate by solid phase epitaxy method under ultra-high vacuum conditions. We measured main Hall parameters. At room temperature, the carrier density was $9.3\times10^{15}$ cm$^{-3}$, the carrier mobility was 327 cm$^2$/(V×s), and resistivity was 2 Ω×cm. It was shown that the used growth mechanism leads to donor behavior of the Ag impurity in contrast with thermal diffusion methods described in literature. The phenomena is caused by occupation of Si sites by Ag atoms.

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