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Research Article

PROPERTIES OF MOLYBDENUM SILICIDE GROWN ON SILICON SINGLE CRYSTALS

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ABSTRACT

This paper presents the properties of compounds of molybdenum silicide Mo - Si. The molybdenum layer was formed with a thickness of 1 ÷ 2 µm by magnetron sputtering onto the surface of a semiconductor from a silicon single crystal grown by the Czochralski method in an atmosphere of pure inert argon gas. The properties of molybdenum silicide formed in the volume of silicon have been studied.

KEYWORDS

Magnetron sputtering, reactive gases, metal, semiconductor, silicide.

INTRODUCTION

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One of the tasks of modern materials science is the creation of new materials with multifunctional coatings [1–3]. Materials with such coatings are widely used in various fields of technology, such as construction, power engineering, microelectronics, aviation, and others [4–7]. Magnetron sputtering is widely used to apply various industrially significant coatings [8]. Such as decorative, wear-resistant or protective coatings with a thickness of several micrometers, and for obtaining complex, multilayer optical structures with layer thicknesses of several tens of nanometers or electrically conductive coatings, the properties and structures of which magnetron sputtering systems allow you to set and vary within the required ranges [9].

Within the framework of this work, they are represented by the introduction of Mo atoms by magnetron ion sputtering on the silicon surface. Using the thermal cycling method to create heat-resistant silicon single crystals, the Mo-Si structure was subjected to thermal heating, where molybdenum atoms migrate deep into the silicon volume. As a result, as studies show, a complex of molybdenum silicide compounds is formed.

The structure of silicide depends on the type of chemical bond between silicon and metal atoms. The silicide of alkali and alkaline earth metals have an ion-covalent bond Mo-Si, the silicide of transition metals have a metal-like bond. In the latter, the interaction between the atoms of the elements is also due to the metallic bond between the metal atoms and the covalent bond between the silicon atoms. The lower the donor ability of the metal, the higher the proportion of the covalent component of the MoSi bond.

Experiment. To obtain a uniform layer of molybdenum Mo, the MSIR method was used by sputtering Mo from a metal target in an inert argon gas medium. The flow rate of the working gases was regulated using RRG-9 gas flow regulators. The pressure in the vacuum chamber was measured using deformation and ionization vacuum gauges. The substrate used was a p- and n-type silicon single crystal with a purity of at least 99.9%, 0.5×1.5 cm in size and 1.4 mm thick. Before coating, the surface of the silicon substrate was cleaned with a cambric cloth with a mixture of polyrite and rectified alcohol diluted in distilled water. After loading the substrates into the working chamber, the surface of the silicon single crystal substrates was subjected to processing using a high-voltage ion source in an argon atmosphere with a 5% oxygen content. The physical thickness of the resulting metal layer was calculated based on the optical thickness $nh=\lambda_0/4$ was 1-2 μm. The film deposition rate (nm/min) was determined based on the physical thickness obtained and the coating time.

According to the equilibrium phase diagram of the Mo-Si state, there are three compounds in this system: molybdenum disilicide $MoSi_2$, lower molybdenum silicides Mo_5Si_3 and Mo_3Si [10]. The solubility of silicon in solid molybdenum is 3.35 at. % at 1820 °C and 9 at. % at 2025 °C. The region of solid solutions based on the Mo_3Si compound is practically absent. There are three eutectics in the system:

- Mo_3Si - Mo_5Si_3 at 26.4 at.% silicon and a temperature of 2020 °C;
- Mo_5Si_3 - $MoSi_2$ at 54 at.% silicon and temperature 1900 °C;
- $MoSi_2$ - Si at 98.5 at.% silicon and a temperature of 1400 °C.

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In addition, according to [11], at a temperature of 1850 °C there is a eutectoid □MoSi2 □ Mo5Si3 + □MoSi2 and at 1900 °C a peritectic □MoSi2 + P □ □MoSi2.

Mo3Si silicide is formed by the peritectic reaction Mo+Si=Mo3Si at 2025±20°C, has a cubic structure with a period a = 0.4890 ± 0.0002. Mo3Si has a close-packed cubic structure or a similar type. The large compactness of the lattice emphasizes the metallic nature of the Mo-Si bond, but there are also covalent bonds between metal atoms in the phases.

According to [12], the homogeneity region of MoSi2 obtained by diffusion saturation in vacuum can be several percent and tends to increase with increasing siliconization temperature. The differences in the concentration of elements are: for Si = 2.52□0.5%; for Mo = 2□0.5%. Silicide MoSi2 undergoes an allotropic transformation in the temperature range 1850 ÷ 1900 °C. The low-temperature variety □-MoSi2 has a tetragonal structure. The high-temperature form □-MoSi2 has a hexagonal structure with parameters: a = 0.4642 ± 0.0005, c = 0.6529 ± 0.0005 nm, c/a - 1.406. The MoSi2 boundary on the Mo side is located at 67.1 ± 1.0% (at.).

The low-temperature form of □-MoSi2 is a tetragonal cell with 2 Mo atoms and 4 Si atoms. Si atoms form a frame, in the voids of which is Mo. The structure can also be considered as consisting of layers parallel to the (010) plane with the closest hexagonal packing. The layers alternate in the order ABAB..., layer B is shifted in the direction of the X axis by a/2. The shortest Mo-Si distance is c/3. Chains of silicon atoms form zigzags passing through Mo prisms parallel to the X and Y axes. a three-dimensional silicon framework is created. The high-temperature form of □-MoSi2 has a hexagonal structure (Table 1).

Table 1. Crystal chemical characteristics of molybdenum silicide's

Compound	Syngonia	Lattice parameters, nm			c/a	X-ray density g/cm^3
		a	b	c		
Mo3Si	cube.	0.4890	-	-		8.968
Mo5Si3	Hex.	0.728	-	0.500	0.69	8.243
Mo5Si3	Tetr.	0.9642	-	0.495	0.5087	8.213
α-MoSi2	Tetr.	0.3203	-	0.7855	2.452	6.267
β-MoSi2	Hex.	0.4642	-	0.6529	1.406	6.26

CONCLUSION

This paper presents magnetron ion sputtering of Mo metal on the surface of a single-crystal silicon semiconductor in an inert argon gas medium. The presence of a small amount of molybdenum silicides in it is able to heal the resulting defects in the structure and facilitates the relaxation of thermal stresses during a sharp change in temperature. With an increase in the operating temperature of structures, silicide compounds in

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the volume of silicon are the main dominant factor in the diffusion dissolution of molybdenum disilicide into metal.

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