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PHYSICOCHEMICAL FOUNDATIONS OF THE FORMATION OF SILICON–METAL COMPOSITE THERMOELECTRIC MATERIALS

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Abstract

This study presents a comprehensive investigation of the physicochemical mechanisms and technological features involved in the formation of silicon-based metal composite materials. Alkali metal atoms were introduced into the silicon crystal lattice using a contact method based on the incorporation of metallic particles, and their interaction with the lattice structure was analyzed in detail. In the subsequent stage, thermal treatment processes were carried out to examine the formation mechanisms of composite phases, diffusion behavior, and structural reorganization phenomena.

The obtained results demonstrate that the spatial distribution of metal atoms, microstructural evolution, and morphological changes significantly influence the thermoelectric and electrical conductivity properties of the material. In addition, it was established that the optimization of doping levels and thermal treatment parameters plays a crucial role in controlling the material properties.

The findings of this research provide an important scientific basis for the development of high-performance silicon-based thermoelectric composite materials, expanding their functional capabilities and enhancing their potential for practical applications.

Keywords

Silicon, composite materials, contact formation via metal particle incorporation, nanocomposite, microstructure, thermoelectric properties, electrophysical properties

Introduction

In recent years, the development of high-efficiency functional materials has become one of the key research directions in thermoelectric materials science. The growing demand for energy efficiency and the utilization of waste heat has significantly increased interest in silicon-based materials [1]. Silicon is distinguished by its technological adaptability, relatively low cost, environmental safety, and widespread application in micro- and nanoelectronics industries.

Unlike conventional monostructured materials, composite and nanocomposite systems possess complex hierarchical architectures, enabling wide-range control over their physical properties. Doping silicon with metal atoms leads to the formation of new phases within the matrix, modification of charge carrier concentration and mobility, and optimization of thermal and electrical transport properties [2]. These factors are essential for enhancing thermoelectric performance. However, the formation of metal–silicon composite systems is associated with several complex scientific and technological challenges, including non-uniform atomic distribution, nonlinear diffusion kinetics, uncontrolled phase transformations, and the need to ensure long-term thermal stability [3]. The aim of this work is to identify the fundamental physicochemical principles governing the formation of silicon-based metal composite structures and to comprehensively evaluate their influence on microstructure, morphology, and functional properties.

Materials and Methods

Silicon granules obtained from recycled raw materials were selected as the object of study. This approach is important from the perspective of developing resource-efficient technologies and improving economic efficiency. Initially, the samples were subjected to mechanical and chemical cleaning processes to ensure surface quality and structural homogeneity.

Alkali and alkaline-earth metal atoms (Na, K, Cs, Ca) were introduced into the silicon matrix using a contact method based on metal particle incorporation [4]. These elements were selected to create donor or acceptor centers in silicon, regulate charge carrier concentration, and promote the formation of composite phases (Fig. 1). The main technological parameters of the implantation process are presented in Table 1.

Table 1

Parameter	**Value / Range**	**Description**
Implantation energy	45 keV	Determines the penetration depth of the atoms
Implantation dose	10^{12}–10^{14} cm^{-2}	Controls the doping level
Introduced elements	Na, K, Cs, Ca	Influences electrical and structural properties
Thermal treatment temperature	300–1000 K	Activates diffusion processes
Vacuum level	~10^{-6} Torr	Prevents oxidation

The impact of incorporated metal atoms on the silicon lattice depends on their physicochemical properties and significantly influences the lattice's electrical, mechanical, and thermal characteristics. Sodium (Na) and potassium (K) atoms exhibit high diffusion activity, enabling facile migration within the lattice. This enhances the material's electrical conductivity by increasing the number of charge carriers [5]. Simultaneously, these atoms slightly modify the internal lattice stresses; however, as predominantly donor species, they contribute electrons, thereby reinforcing the semiconducting properties. Cesium (Cs) atoms, due to their large ionic radius, alter the geometry of the silicon lattice and induce lattice deformation. This affects the lattice's elastic properties, slightly expanding the structure and increasing its flexibility. Calcium (Ca) atoms form relatively stable compounds, thereby enhancing the mechanical strength of the composite phase. They also contribute to the long-term stability of the lattice, improving its resistance to thermal and mechanical stress.

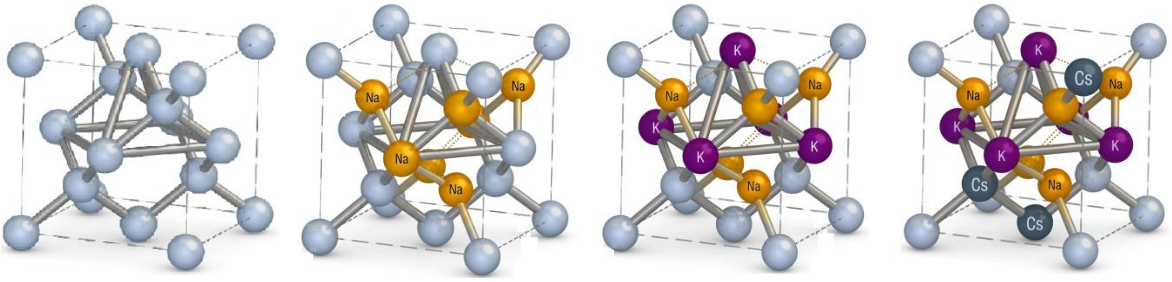

Figure 1. Distribution of alkali metals in the silicon crystal lattice

The samples containing metal particles were initially subjected to contact implantation, followed by thermal treatment under high vacuum conditions at temperatures ranging from 300 to 1000 K. During this stage, diffusion processes were activated, allowing the defects introduced during implantation to reorganize and facilitating the formation of metal–silicon composite phases. Thermal treatment also promoted the migration mechanisms of charge carriers within the material, leading to the redistribution of electrons and ions. As a result, the electrical, thermal, and mechanical properties of the material were modified, and a stable composite structure was formed [6].

In the subsequent stage, the samples were mechanically dispersed to achieve a powder form with particle sizes of 0.5–1.0 µm. This process significantly increased the surface area and enhanced the material's reactivity. Consequently, the samples were optimized for further experimental studies, allowing for easier analysis of modifiable phases and diffusion processes.

When copper (Cu), nickel (Ni), and iron (Fe) atoms were incorporated into the silicon lattice, each element exerted a distinct influence on the properties of the resulting composite material (Figure 2). Copper atoms, characterized by facile electron exchange and small ionic radius, increased the electron density of the composite lattice. This significantly improved conductivity in semiconductor materials and slightly enhanced the mechanical rigidity of the composite structure, without substantially affecting deformation resistance [7].

Nickel atoms strongly influenced the thermal and mechanical properties of the composite. Due to its relatively stable electronic configuration, nickel enhanced the lattice's resistance to deformation and improved overall structural stability. Additionally, nickel's electron-donating capability supported the semiconductor properties, although the increase in electrical conductivity was lower than that of copper.

Iron atoms contributed additional mechanical strength to the composite lattice and reduced internal stresses. Furthermore, iron increased the thermal resistance of the composite material and ensured long-term stability. Through its electron-donating effect, iron slightly enhanced the semiconducting properties, although its impact on conductivity was less pronounced compared to copper and nickel.

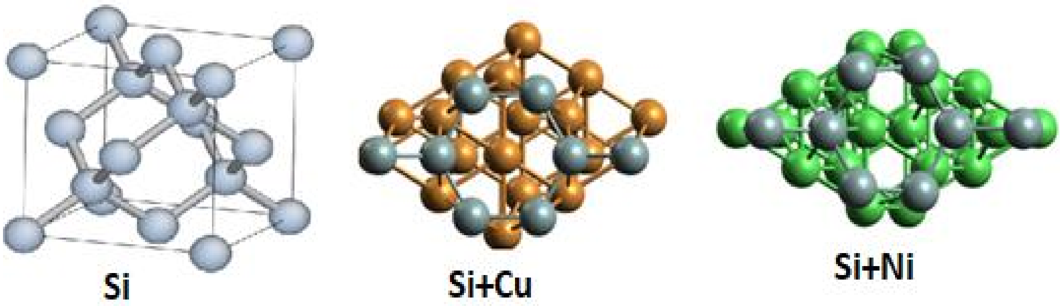

Figure 2. Distribution of transition metals in the silicon crystal lattice

Overall, the silicon composite lattice formed with copper, nickel, and iron exhibits a synergistic enhancement of electrical, mechanical, and thermal properties, enabling the development of high-performance materials suitable for various functional and industrial applications.

Results and Discussion

The conducted study provided a comprehensive analysis of the formation mechanisms and functional properties of silicon-based thermoelectric composite materials and contacts. Experimental results indicate that the incorporation of metal atoms into the silicon matrix leads to significant refinement of the microstructure, increased dispersion, and the formation of nanoscale composite phases. This process is directly linked to mechanical dispersion and subsequent thermal treatment, resulting in an increased surface area and enhanced material reactivity. Moreover, the resulting hierarchical structure plays a crucial role in improving thermoelectric properties.

Analysis of samples alloyed with alkali and alkaline-earth metals (Na, K, Cs, Ca) revealed that Na and K atoms, due to their high diffusion activity, rapidly migrate throughout the lattice, increasing the concentration of charge carriers. This results in a substantial enhancement of electrical conductivity. Cs atoms, having a large ionic radius, induce lattice distortion and modify elastic properties [8]. The presence of Ca leads to the formation of relatively stable composite phases, improving both the mechanical strength and thermal stability of the material.

These processes also increase the number of energetically active centers on particle surfaces, contributing to enhanced thermoelectric efficiency (Figure 3).

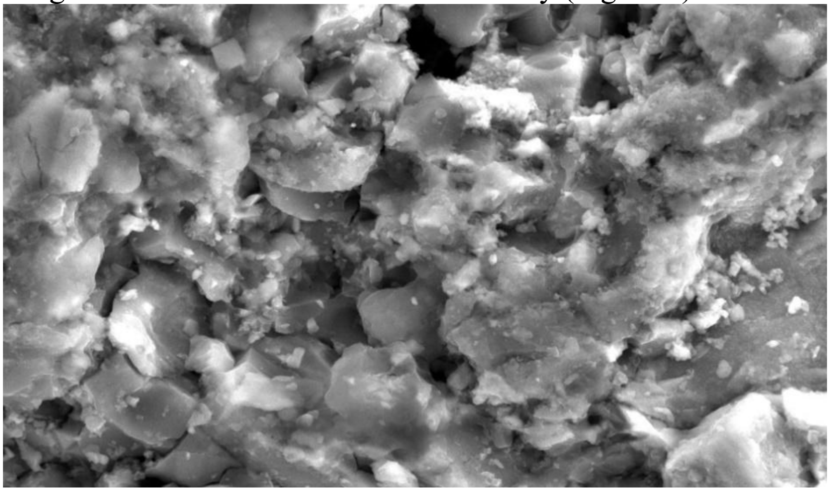

Figure 3. Microstructure of silicon-based composite material

The incorporation of transition metal atoms (Cu, Ni, Fe) further complicates and optimizes the properties of the composite system. Copper atoms act as electron donors, increasing electron density and significantly enhancing the electrical conductivity of the material. Nickel atoms contribute to structural stability, improve resistance to deformation, and enhance thermal stability under heat exposure. Iron atoms reduce internal stresses, increase mechanical strength, and improve heat resistance. Moreover, the synergistic combination of these metals promotes the formation of new functional phases within the composite material.

During thermal treatment at 300–1000 K, diffusion and recrystallization processes intensify, resulting in the redistribution of atoms and the transition from metastable to stable phases. This ensures uniform distribution of metal atoms within the silicon matrix and enhances the stability of the composite structure. Consequently, both electrical and thermal transport properties of the material are improved(Figure 4).

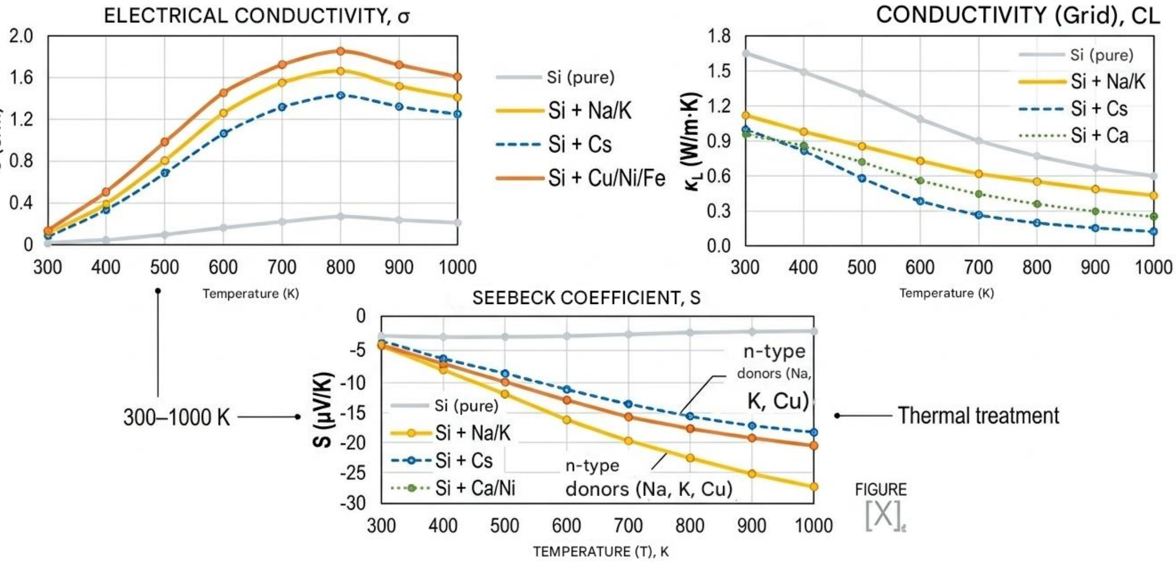

Figure-4. Temperature Dependence of Thermoelectric Parameters

The results indicate that high-efficiency thermoelectric contacts can be fabricated using multi-component silicon-based composite materials. By controlling the type and concentration of metal atoms as well as thermal treatment parameters, it is possible to deliberately modify the microstructure and functional properties of the material. This approach holds significant scientific and practical importance for the development of modern energy-saving technologies and waste heat recovery systems.

Conclusion

This study focused on elucidating the physicochemical mechanisms governing the formation of silicon-based metal–composite thermoelectric materials and optimizing their functional properties. The results demonstrated that the incorporation of metal particles via contact implantation followed by thermal treatment is a crucial technological factor in controlling the formation of composite phases.

Alloying with alkali and alkaline-earth metals (Na, K, Cs, Ca) activates diffusion processes within the silicon matrix, increasing the concentration of charge carriers. Specifically, Na and K atoms, due to their high diffusivity, significantly enhance electrical conductivity, while Cs atoms induce lattice deformation, affecting structural characteristics. Ca atoms contribute to the formation of stable composite phases, improving the mechanical strength and thermal stability of the material.

The addition of transition metals (Cu, Ni, Fe) further optimizes the functional properties of the composite system. Copper atoms, acting as electron donors, enhance electrical conductivity; nickel improves structural stability and resistance to deformation; and iron increases mechanical strength and thermal stability. The synergistic effect of these elements promotes the formation of new functional composite phases. Grain refinement, increased dispersity, and the formation of nanoscale phases enhance the surface properties and increase the number of energetically active centers. During thermal treatment at 300–1000 K, accelerated diffusion and recrystallization ensure uniform atom distribution and transition from metastable to thermodynamically stable phases. By optimizing alloying levels, metal types, and thermal processing parameters, it is possible to precisely control the thermoelectric, electrical, and mechanical properties of silicon-based composite materials.

These findings provide a scientific foundation for developing high-efficiency thermoelectric composite contacts and advancing energy-saving technologies.

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