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DIFFUSION DISTRIBUTION OF Cr AND Mn IMPURITY ATOMS IN SILICON

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This work presents theoretical calculations of the diffusion coefficient, solubility, and diffusion distribution of Mn and Cr impurity atoms in silicon. The results of theoretical studies showed that the distribution of Cr element atoms in silicon is slightly different from the distribution of Mn element atoms in silicon, while the remaining physical and chemical properties are almost identical. Also, if a Mn atom is placed at a node in a silicon single crystal, it will have three charge states: neutral – Mn^0, one electron lost – Mn^{+1}, and two electrons lost – Mn^{+2}. Similarly, if a Cr atom is placed at the node of a silicon single crystal, it will have four different charge states: neutral – Cr^0, one electron lost – Cr^{+1}, two electrons lost – Cr^{+2}, and three electrons lost – Cr^{+3}. Therefore, it is relevant to study the properties of doped silicon with Cr impurity atoms.
Keywords: *Silicon; Impurity atoms; Diffusion; Manganese; Chromium; Distribution*
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1. INTRODUCTION

It is known that in the Si semiconductor, B, Al, In, and Ga impurities form acceptor energy levels, and P, Sb, and As impurities form donor energy levels. These inclusions have high solubility ($N_{III,V}$~10^{19}÷10^{21} cm^{-3}) in Si semiconductor, but their diffusion coefficients ($D_{III,V}(T)$~10^{-14}÷10^{-11} cm^2/s) are very small [1-4]. Group III and V elements are doped into the Si semiconductor to form a *p-n* structure to develop various electronic devices such as solar cells, semiconductor diodes, and transistors [5-8]. It is very difficult to doped group III and V elements through the entire thickness of a Si sample by diffusion. Therefore, it is not possible to obtain strongly compensated Si using these impurities. Also, almost 100% of the atoms of elements of groups III and V are located at the crystal lattice node of the Si semiconductor and participate in sp^3 hybrid bonding. Therefore, magnetic properties are not observed in Si samples doped with group III and V elements.

It is known from the authors' work that the magnetic properties of the Si semiconductor are mainly formed as a result of doping with *d* and *f* group elements [9-11]. The use of electron spin in semiconductor devices opens up a new area of potential applications in high-speed, low-power spintronic devices [12-14]. One of the main research areas in this field is ferromagnetic semiconductors, which are created by magnetic and electrical doping of classical semiconductor materials [15,16]. Determining the ferromagnetic properties of Si, the most important material in the electronics industry, is important. To this end, many scientists are conducting theoretical and practical research. The electronic configuration of the element Mn is $1s^22s^22p^63s^23p^63d^54s^2$, the electronic configuration of the element Cr is $1s^22s^22p^63s^23p^63d^54s^1$, and these elements are *d* group elements, and their physical and chemical properties are very similar to each other. Therefore, this work is devoted to theoretical calculations of the distribution of charge carriers in silicon doped with Mn and Cr impurity atoms.

2. THEORETICAL PART

2.1. Charge carrier distribution

It is known that diffusion is divided into diffusion from a finite (1) [17] and an infinite (2) [17] source, depending on the ratio of the amount of impurity and the solubility in the semiconductor. The diffusion distribution of impurity atoms is calculated using the following function:

$$C(T) = C_0 \cdot \exp\left(\frac{-x^2}{4 \cdot D \cdot t}\right) \quad (1)$$

$$C_\infty(T) = C_0 \cdot erfc\left(\frac{x}{2\sqrt{D \cdot t}}\right) \quad (2)$$

where, x – is the depth of penetration of the impurity atoms into the crystal, D – is the diffusion coefficient, t – is the diffusion time, C_0 – is the maximum solubility of the impurity atoms in the crystal at temperature T, $C(T)$ (from a finite source) and $C_\infty(T)$ (from an infinite source) are the concentrations of the impurity atoms, $erfc(\eta)$ – is the Gaussian error function, and η – is the argument of the Gaussian error function.

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Therefore, to calculate the diffusion distribution of impurity atoms in silicon, we need to determine the temperature dependence of the diffusion coefficient, the temperature dependence of the maximum solubility of impurity atoms, and the Gaussian error function.

2.2. Diffusion coefficient

The diffusion coefficient is determined using the following expression (3):

$$D(T) = D_0 \cdot \exp\left(-\frac{E_a}{kT}\right) \tag{3}$$

where E_a – is the activation energy, k – is the Boltzmann constant, D_0 – is the diffusion constant at infinite temperature, and T – is the absolute temperature.

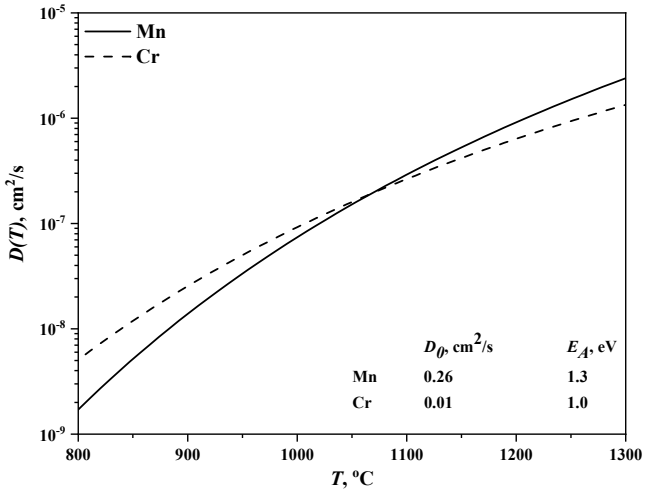

Figure 1. Diffusion coefficient of Mn and Cr impurity atoms in silicon.

From Figure 1, it can be seen that $D_{Cr} > D_{Mn}$ up to temperatures $T_1 < 1050$ °C, $D_{Cr} \approx D_{Mn}$ in the temperature range 1050 °C$\leq T_2 \leq$1100 °C, and $D_{Cr} < D_{Mn}$ at temperatures above $T_3 > 1100$ °C.

2.3. Solubility of impurity atoms

The temperature dependence of the maximum solubility of impurity atoms in a crystal is determined by the following formula:

$$N(T) = N_0 \cdot \exp\left(-\frac{E_s}{k \cdot T}\right) \tag{4}$$

where N_0 – is a quantity equal to the maximum solubility of the impurity atoms at infinitely high temperature, and E_s – is the solubility energy.

From Figure 2, it can be seen that the solubility of Mn and Cr impurity atoms in silicon is almost equal to each other.

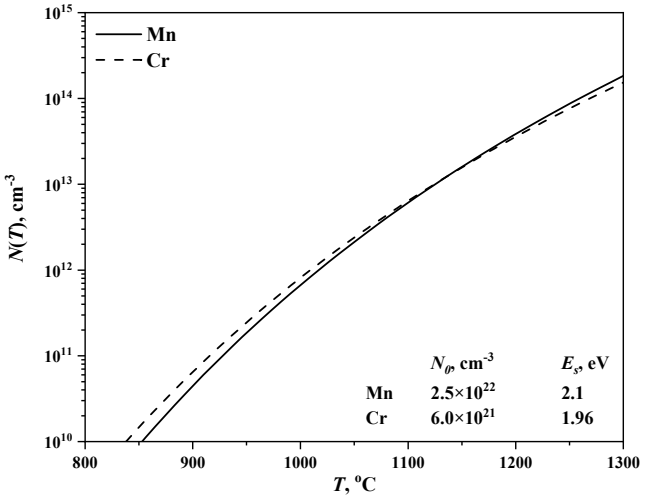

Figure 2. Solubility of Mn and Cr impurity atoms in silicon

2.4. Gaussian error function

The Gaussian error function is defined using the following expression:

$$erfc(\eta) = 1 - erf(\eta), \tag{5}$$

$$erf(\eta) = \frac{2}{\sqrt{\pi}} \int_0^x \exp\left(-\eta^2\right) dt, \tag{6}$$

$$erfc(\eta) = 1 - \frac{2}{\sqrt{\pi}} \int_0^x \exp\left(-\eta^2\right) dt. \tag{7}$$

Figure 3 depicts the graph of the relationship $erf(\eta) = f(\eta)$, which can be used in calculations.

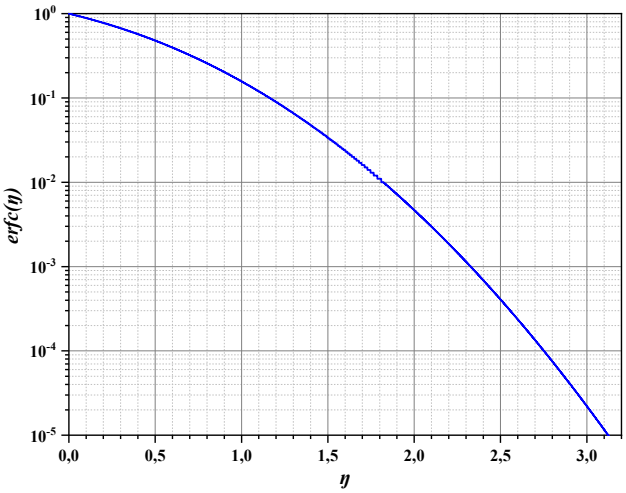

Figure 3. Gaussian error function ($erf(\eta)$) as a function of its argument (η)

3. RESULTS OF THEORETICAL CALCULATION

In the works of the authors [18,19], the diffusion process of Mn impurity atoms into Si was carried out in the temperature range T~1000÷1100 °C. Based on the above data, the diffusion distribution of Mn and Cr impurity atoms in Si was calculated in the temperature range T~950÷1150 °C (Figure 5 and Figure 6).

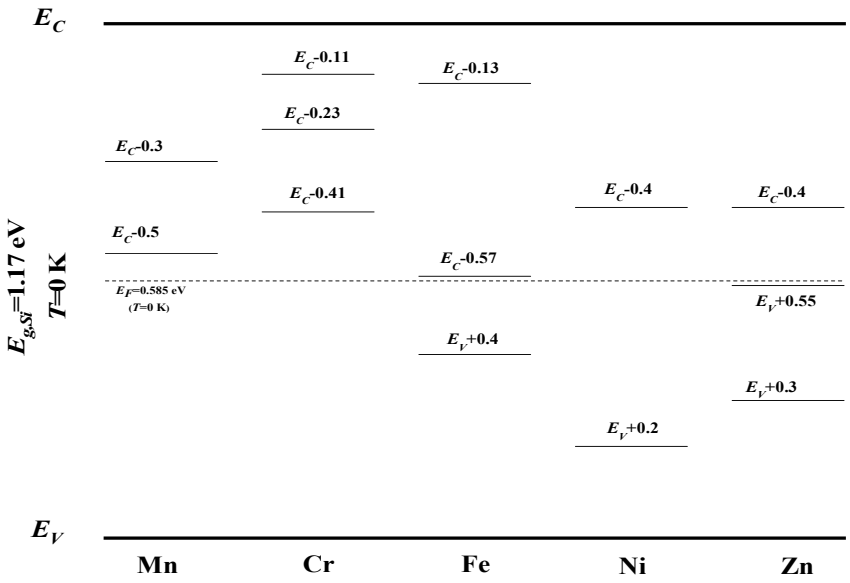

Figure 4. Energy levels of some elements in silicon.

It is known that Mn impurity atoms form two donor energy levels E_C–0.3 eV and E_C–0.5 eV in silicon [20] (see Figure 4). Cr impurity atoms form three donor energy levels in silicon, E_C–0.11 eV, E_C–0.23 eV, and E_C–0.41 eV [20] (see Figure 4). As can be seen from figure 4, when a Mn impurity atom is placed at a node of a silicon single crystal, it will have three charge states: neutral–Mn^0, one electron lost–Mn^{+1}, and two electrons lost–Mn^{+2}. Similarly, if Cr

impurity atoms is placed at the node of a silicon single crystal, it will have four different charge states: neutral – Cr^0, one electron lost – Cr^{+1}, two electrons lost – Cr^{+2}, and three electrons lost – Cr^{+3}.

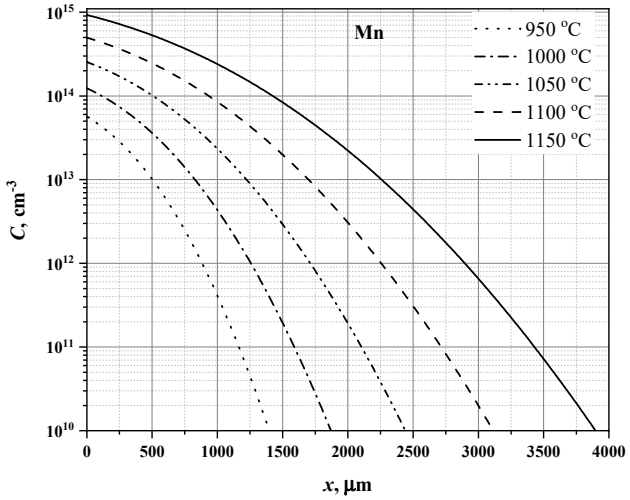

Figure 5. Diffusion distribution of Mn dopant atoms in silicon calculated using equations (2), (3) and (4)

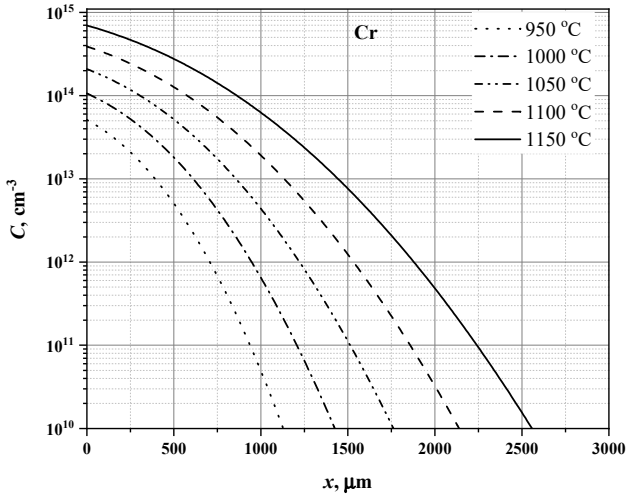

Figure 6. Diffusion distribution of Cr dopant atoms in silicon calculated using equations (2), (3) and (4)

4. CONCLUSION

Currently, many scientists have studied the magnetic properties of silicon doped with Mn [9-20] impurity atoms, while the magnetic properties of silicon doped with Cr [21] impurity atoms have been less studied. Theoretical calculations show that the diffusion coefficients of Mn and Cr impurity atoms in silicon (Figure 1) and maximum solubility (Figure 2) are very close to each other, but their electronic configurations and distribution in silicon (Figures 5 and 6) are slightly different. Therefore, it requires a lot of theoretical and practical research to study the electrical-physical, electromagnetic, magnetic, optical, photoelectric, and magneto-photonic properties of a Si sample doped with Cr impurity atoms.

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ДИФУЗІЙНИЙ РОЗПОДІЛ ДОМІШКОВИХ АТОМІВ Cr ТА Mn У КРЕМНІЇ

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У роботі наведено теоретичні розрахунки коефіцієнта дифузії, розчинності та дифузійного розподілу домішкових атомів Mn і Cr у кремнії. Результати теоретичних досліджень показали, що розподіл атомів елемента Cr у кремнії дещо відрізняється від розподілу атомів елемента Mn у кремнії, а решта фізико-хімічних властивостей майже ідентичні. Крім того, якщо атом Mn помістити у вузол монокристалу кремнію, він матиме три зарядові стани: нейтральний – Mn^0, один втрачений електрон – Mn^{+1} і два втрачені електрони – Mn^{+2}. Подібним чином, якщо атом Cr помістити у вузол монокристала кремнію, він матиме чотири різні стани заряду: нейтральний – Cr^0, один втрачений електрон – Cr^{+1}, два втрачені електрони – Cr^{+2} і три втрачені електрони – Cr^{+3}. Тому актуальним є дослідження властивостей легованого кремнію домішковими атомами Cr.

Ключові слова: *кремній; домішкові атоми; дифузія; марганець; хром; розподіл*