MECHANISMS OF PIEZORESISTIVITY IN COMPENSATED SILICON WITH DEEP-LEVEL IMPURITIES UNDER HYDROSTATIC PRESSURE

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Keywords: *compensated silicon, deep-level impurities, hydrostatic pressure, piezoresistivity, carrier transport, deformation potential, deep-level shift*

Abstract: *This study investigates the mechanisms of the piezoresistive effect (tensoeffect) in compensated silicon doped with deep-level impurities (Mn, Ni, Gd) under the influence of all-round hydrostatic compression. The research addresses the problem of interpreting changes in electrical conductivity, which are often ambiguous under isotropic deformation due to the simultaneous variation of carrier concentration and mobility. The applied methodology involves the development of a theoretical model based on the analysis of provided experimental data for n- and p-type Si<Ni> and Si<Mn>. The model accounts for pressure-induced shifts of deep impurity levels and the conduction/valence band edges, which alter the ionization degree of scattering centers and the free carrier concentration. Key results include the quantitative determination of the baric coefficient for the ionization energy of the Mn level ($\alpha \approx 1.81 \cdot 10^{-11}$ eV/Pa) and for Ni/Gd levels ($\alpha \approx -0.7 \cdot 10^{-11}$ and $-0.8 \cdot 10^{-11}$ eV/Pa, respectively). It is shown that in Si<Mn>, the piezoresistive effect is primarily governed by changes in carrier concentration, while in Si<Ni>, the redistribution of carriers between deep levels and bands, along with the influence of potential barriers*

from Ni precipitates, plays a decisive role. The main conclusion is that the piezoresistive response in heavily compensated silicon under hydrostatic pressure is dominantly controlled by the electronic properties of deep-level impurities and related structural inhomogeneities, rather than by intervalley scattering mechanisms [1]. This provides a foundation for the development of sensitive pressure sensors based on compensated semiconductor structures.

Introduction

The study of semiconductors under high pressure is a powerful tool for investigating their electronic structure, defect properties, and charge transport mechanisms. The piezoresistive effect, a change in electrical resistance upon mechanical deformation, is of fundamental importance for both understanding material physics and developing sensor applications. In silicon, the effect is well-studied for uniaxial stress, where it is strong due to the anisotropy of the conduction and valence bands. However, under isotropic hydrostatic compression, which preserves crystal symmetry, the classical mechanisms related to band degeneracy lifting are suppressed, making the interpretation of resistivity changes more complex [1]. This complexity is especially pronounced in compensated semiconductors containing deep-level impurities, where electrical properties are highly sensitive to defect states and structural inhomogeneities. This work aims to fill the specific scientific gap concerning the dominant physical mechanisms governing the piezoresistive response in heavily compensated silicon with transition metal impurities (Ni, Mn, Gd) under all-round hydrostatic pressure, a regime where standard models are insufficient.

The classical theory of piezoresistance in silicon relates it primarily to changes in carrier mobility due to altered scattering rates and effective masses under anisotropic deformation. Under hydrostatic pressure, the equivalence of conduction band valleys in silicon is not broken, theoretically eliminating the contribution from intervalley scattering [1]. Prior research on p-type silicon doped with boron (p-Si<B>) has confirmed a weaker piezoresistive effect under all-round compression

compared to uniaxial stress [6]. Some mobility increase observed in p-Si<B> was attributed to an upward shift of the valence band maximum, reducing hole energy [1]. For materials with deep-level impurities, the situation is less clear. It is established that clusters of impurities like Mn in compensated Si<Mn> create a static, spatially inhomogeneous electric potential of large amplitude [2]. Furthermore, post-thermal treatment of silicon can lead to the formation of microdefects and impurity clouds that act as scattering centers [5]. Studies on nickel in silicon indicate that Ni atoms can form precipitates, creating regions of crystalline distortion and high concentrations of electrically active defects that compensate shallow dopants and form potential barriers [3]. These findings suggest that in compensated materials, pressure-induced changes in the occupation of deep levels and the modification of potential landscapes around defects and precipitates may be key to understanding piezoresistance under hydrostatic conditions. Hall effect studies under pressure for Si<Mn> have provided direct data on carrier concentration changes [4].

Theoretical Framework and Modeling

To explain the experimental observations, a model is developed focusing on the pressure-induced shift of deep impurity levels relative to the band edges. This shift changes the ionization equilibrium, affecting both free carrier concentration and the charge state of scattering centers. For a deep donor level (e.g., Mn in n-Si), the electron concentration under pressure P can be described by:

$$n = n_0 \cdot \exp\left(-\frac{E_d - \alpha P}{kT}\right) \quad (1)$$

where n_0 is the equilibrium concentration at P=0, E_d is the ionization energy of the deep level at zero pressure, \alpha is the baric coefficient for the ionization energy change, k is Boltzmann's constant, and T is temperature. Equation (1) directly links the change in carrier concentration to the pressure-dependent shift of the defect level. The baric coefficient \alpha can be determined experimentally by comparing carrier concentrations at two different pressures, P_1 and P_2:

$$\alpha = \frac{kT}{\Delta P} \ln\left(\frac{n(P_2)}{n(P_1)}\right) \quad (2)$$

where $\Delta P = P_2 - P_1$. The change in carrier mobility \mu is modeled considering scattering on ionized impurities. The scattering potential and, consequently, the mobility, depend on the concentration of ionized centers N_i .*Under pressure,* N_i changes due to the shift of the Fermi level and deep levels. For n-type material with deep donors, de-ionization under pressure reduces N_i, *potentially increasing mobility. Conversely, in p-type material with deep centers acting as electron traps, an increase in hole concentration can lead to a higher degree of center ionization (via electron capture from the valence band), increasing* N_i and thus reducing hole mobility. This framework allows for the separation of effects stemming from pure carrier concentration changes (related to \alpha) and those from mobility changes (related to the variation of N_i^*).

Analysis of Experimental Data and Discussion

The analysis of data for n-Si<Mn> reveals that the application of hydrostatic pressure (up to $5 \cdot 10^8$ Pa) increases the electron concentration, as seen in the Hall effect measurements presented in the form ln n = f(10^3/T) [4]. Processing this data using equation (1) yields a baric coefficient $\alpha_{Mn} \approx 1.81 \cdot 10^{-11} eV/Pa$, indicating a decrease in the Mn level ionization energy under pressure. The concurrent decrease in electron mobility is attributed to the increased concentration of ionized Mn scattering centers, which is consistent with the model of an inhomogeneous potential created by Mn clusters [2], despite the overall rise in free electron concentration. This confirms that the piezoresistive effect in Si<Mn> is primarily governed by carrier concentration changes.

For Si<Ni>, the situation involves additional complexity. The significant decrease in carrier mobilities (to 600–700 $cm^2/V \cdot s$ for electrons and 60–100 $cm^2/V \cdot s$ for holes in heavily compensated samples) after diffusion annealing points to the formation of strong scattering centers, likely Ni precipitates and associated defect clouds as described in [3]. Under hydrostatic pressure, the model suggests a decrease in the ionization energy of Ni-related and other uncontrolled impurity levels. In n-Si<Ni>, this leads to an increase in free electron concentration and a decrease in the

ionization degree of scattering centers. Both effects—de-ionization and increased screening by free electrons—contribute to the observed increase in electron mobility. In p-Si<Ni>, however, the increase in hole concentration enhances the ionization of centers (as electrons are captured onto them from the valence band), increasing the scattering potential and thus reducing hole mobility. Calculations based on equation (2) and the experimental data yield baric coefficients $\alpha_{Ni} \approx -0.7 \cdot 10^{-11} eV/Pa$ and $\alpha_{Gd} \approx -0.8 \cdot 10^{-11} eV/Pa$. The negative sign indicates a reduction in the ionization energy gap under pressure. This analysis underscores the decisive role of deep-level recharge kinetics and the inhomogeneous potential landscape created by precipitates in Si<Ni> [3]. The behavior contrasts with that of p-Si<B>, where the effect under hydrostatic pressure is weaker and governed by different mechanisms [1, 6].

Conclusion

This research elucidates the fundamental mechanisms behind the piezoresistive effect in heavily compensated silicon doped with deep-level impurities (Mn, Ni) under hydrostatic pressure. It is demonstrated that the classical mechanism related to intervalley scattering is negligible in this isotropic regime [1]. Instead, the effect is dominated by pressure-induced shifts of deep impurity levels, which drastically alter the equilibrium between free carriers and charged scattering centers. For Si<Mn>, the effect is primarily a consequence of changing carrier concentration, linked to the specific baric coefficient of the Mn level [2, 4]. For Si<Ni>, the response is more complex, involving a interplay between level shifts, carrier redistribution, and scattering on potential barriers associated with Ni precipitates [3]. The quantitative determination of baric coefficients for the ionization energy of Mn, Ni, and Gd levels provides key parameters for modeling such systems. These findings advance the understanding of charge transport in disordered semiconductor systems under mechanical stress and suggest pathways for engineering silicon-based materials with tailored piezoresistive properties for advanced sensor applications.

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