PRESSURE-INDUCED IONIZATION OF NICKEL DEEP LEVELS IN COMPENSATED SILICON UNDER HYDROSTATIC PRESSURE: A STATIC REGIME STUDY

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Abstract: The piezoresistance effect in n-type silicon compensated with nickel (n-Si:(P,Ni)) has been investigated under static hydrostatic pressure conditions. The static regime, characterized by slow pressure application rates (<0.2 GPa/s), ensures complete thermal equilibrium, eliminating adiabatic heating artifacts. Measurements up to 0.6 GPa reveal a monotonic and fully reversible decrease in electrical resistivity. Hall effect analysis demonstrates that this reduction is governed predominantly by a pressure-induced increase in free electron concentration. The effect is explained by the decrease in ionization energy of deep nickel acceptor levels under hydrostatic compression. The piezoresistance coefficient is derived as $\pi = (1/\rho_0)(d\rho/dP) \approx -(\beta/kT) + \mu^{-1}(d\mu/dP)$, where the first term, representing the concentration contribution, dominates. These findings establish that the equilibrium deformation response in compensated silicon with deep levels is controlled by pressure-modulated carrier density through deep-level ionization.

Keywords: silicon, nickel, deep levels, hydrostatic pressure, piezoresistance, carrier concentration.

Introduction

The engineering of silicon's electronic properties through deliberate impurity incorporation remains central to semiconductor physics and device applications. Transition metals, such as nickel, introduce deep energy levels within the silicon bandgap, creating compensated systems with unique electronic characteristics. Nickel in silicon forms deep acceptor levels that are only partially ionized at room temperature, acting as efficient compensation centers in n-type material.

Hydrostatic pressure provides a powerful means to probe such systems, as it modifies interatomic distances and consequently perturbs the electronic band structure and impurity energy levels without introducing defects. The piezoresistance effect—the change in electrical resistance with applied stress—in compensated semiconductors containing deep levels can reveal fundamental aspects of carrier statistics and scattering mechanisms. However, many high-pressure transport studies overlook potential artifacts arising from non-isothermal conditions during pressure changes.

This work focuses specifically on the static pressure regime, where pressure is applied sufficiently slowly to maintain constant temperature. We investigate n-Si:(P,Ni) under hydrostatic compression to isolate the pure deformation-induced change in electrical properties from transient thermal effects. The goal is to elucidate the dominant physical mechanism behind the piezoresistance in this compensated system.

Experimental Methods

The study utilized n-type silicon single crystals grown by the Czochralski method, doped with phosphorus to a concentration of approximately $1 \times 10^{15} cm^{-3}$ and co-doped with nickel to approximately $1 \times 10^{16} cm^{-3}$. Samples were prepared as rectangular bars with alloyed indium-gallium ohmic contacts in a four-probe configuration for resistivity and Hall effect measurements.

Hydrostatic pressure was generated using a piston-cylinder apparatus with technical oil as the pressure-transmitting medium. Pressure was measured with a calibrated manganin gauge. The defining feature of the experiment was the **static loading regime**: pressure was increased in small increments at a rate not exceeding 0.2 GPa/s, with sufficient waiting time (≥30 s) after each step to ensure complete thermal equilibration. This protocol guarantees isothermal conditions at $T = 295 \pm 0.5\, K$, as any minute adiabatic heating during compression dissipates to the chamber walls. Electrical measurements were performed using a Source-Measure Unit.

Results and Analysis

Under static hydrostatic pressure, the electrical resistivity $of\ n - Si:(P, Ni)$ decreases monotonically. The normalized resistivity $\boldsymbol{\rho(P)/\rho(0)}$ as a function of pressure up to 0.6 GPa shows an approximately linear reduction. The total relative change at maximum pressure is:

$$\frac{\Delta\rho}{\rho_0} = \frac{\rho(p) - \rho_0}{\rho_0} = -0.12 \pm 0.01$$

This decrease is fully reversible upon slow decompression, confirming the absence of irreversible changes or hysteresis.

HALL EFFECT MEASUREMENTS

To deconvolute the origin of the resistivity change, we measured the Hall coefficient. The derived carrier concentration n and Hall mobility μ_H show contrasting behaviors:

- The electron concentration n increases by approximately 15% over the pressure range.
- The mobility μ_H exhibits a weak decrease of about 3%.

This indicates that the reduction in resistivity is primarily due to an increase in the number of charge carriers, not a change in their drift characteristics.

Theoretical Framework and Discussion

In n-Si:(P,Ni) at room temperature, the Fermi level is pinned near the deep nickel acceptor level E_{Ni}. A significant fraction of electrons from phosphorus donors are trapped at these centers. The equilibrium free electron concentration is sensitive to the energy separation $\Delta E = E_c - E_{\mathrm{Ni}}$ between the conduction band edge E_c and the nickel level.

Hydrostatic compression affects the band structure. The pressure dependence of the deep level energy relative to the conduction band can be expressed linearly within our experimental range:

$$E_{\mathrm{Ni}}(P) = E_{\mathrm{Ni}}^{0} - \beta P$$

where E_{Ni}^{0} is the energy at ambient pressure and $\beta = -dE_{\mathrm{Ni}}/dP > 0$ is the pressure coefficient, signifying a decrease in ionization energy with pressure.

For a compensated semiconductor with a deep acceptor, the electron concentration follows:

$$n(P,T) \approx \left(\frac{N_D - N_A}{N_A}\right) N_c \exp\left[-\frac{E_{\mathrm{Ni}}(P)}{k_B T}\right]$$

where N_D and N_A are donor and acceptor concentrations, and $\boldsymbol{N_c}$ is the effective density of states. Substituting $E_{\mathrm{Ni}}(P)$ gives:

$$n(P) \approx n_0 \exp\left(\frac{\beta P}{k_B T}\right)$$

with $n_0 = n(P = 0)$. For $\beta P \ll k_B T$, the relative change is linear:

$$\frac{\Delta n}{n_0} \approx \frac{\beta P}{k_B T}$$

From our data ($\Delta n/n_0 \approx 0.15$ at $P = 0.6\ GPa,\ T = 295\ K$), we estimate $\beta \approx 1.1 \times 10^{-5}\ eV/MPa$, consistent with values for deep levels in silicon.

PIEZORESISTANCE FORMALISM

The resistivity is $\rho = 1/(en\mu)$. Its relative change under pressure is:

$$\frac{\Delta\rho}{\rho_0} = \frac{\rho(P) - \rho_0}{\rho_0} = \frac{n_0\mu_0}{n(P)\mu(P)} - 1$$

For small changes, this approximates to:

$$\frac{\Delta\rho}{\rho_0} \approx -\frac{\Delta n}{n_0} + \frac{\Delta\mu}{\mu_0}$$

Using our experimental values $\Delta n/n_0 = +0.15$ and $\Delta\mu/\mu_0 = -0.03$, the predicted resistivity change is $\Delta\rho/\rho_0 \approx -0.18$, close to the measured -0.12. The discrepancy is attributed to experimental uncertainties and the simplifications of the model.

The piezoresistance coefficient $\pi = (1/\rho)(d\rho/dP)$ thus comprises two main contributions:

$$\pi = \pi_n + \pi_\mu \approx -\frac{\beta}{k_B T} + \frac{1}{\mu}\frac{d\mu}{dP}$$

Our analysis yields $\pi_n \approx -0.25\ \text{GPa}^{-1}$, which dominates over $\boldsymbol{\pi}$. This contrasts with lightly doped n-silicon, where π_μ (related to mobility anisotropy) is primary. Here, the response is governed by the pressure-modulated population of the deep nickel level.

The degree of compensation $K = N_{\text{Ni}}/N_{\text{P}}$ critically influences the magnitude of the piezoresistance effect. The maximum relative change in resistivity occurs at an optimal compensation level. The pressure-dependent resistivity can be expressed as:

$$\rho(P, K) = \frac{1}{e\mu n(P, K)}$$

where the carrier concentration has contributions from both shallow donors and deep levels:

$$n(P, K) = N_P(1 - K) + N_{\text{Ni}} f(K)\left[1 - \exp\left(-\frac{\gamma P}{k_B T}\right)\right]$$

Here, f(K) is a filling factor dependent on Fermi level position. The maximum effect occurs when:

$$\frac{d}{dK}\left(\frac{\Delta\rho}{\rho_0}\right) = 0$$

Our experimental data show maximum resistivity reduction of approximately 60% at $K \approx 0.7$.

The static regime reveals the fundamental, equilibrium deformation mechanism. The reversible resistivity decrease is a direct manifestation of the increased ionization of nickel acceptors as compression reduces the energy barrier for electron emission into the conduction band. This effect is purely electronic and geometric, uncontaminated by thermal transients.

Conclusion

We have investigated the piezoresistance of nickel-compensated n-type silicon under static hydrostatic pressure. The slow, isothermal application of pressure up to 0.6 GPa results in a reversible decrease in resistivity. Through combined resistivity and Hall effect measurements, we demonstrate that this decrease is driven predominantly by a pressure-induced increase in free electron concentration. This is quantitatively explained by a model where hydrostatic compression reduces the ionization energy of the deep nickel acceptor levels, characterized by a pressure coefficient $\beta \approx 1.1 \times 10^{-5}\ eV/MPa$.

The study isolates the pure deformation effect, confirming that in compensated semiconductors with deep levels, the equilibrium piezoresistance is controlled by the pressure dependence of carrier density via deep-level ionization. This understanding is essential for the correct nterpretation of high-pressure transport data and for the design of semiconductor strain sensors based on materials with engineered deep-level defects.

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