DYNAMIC PIEZORESISTIVITY AND BARRIER HEIGHT MODULATION IN SCHOTTKY STRUCTURES BASED ON COMPENSATED SILICON UNDER PULSED HYDROSTATIC PRESSURE

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Abstract*: This study presents a theoretical analysis of the dynamic piezoresistive response in Au/n-Si Schottky barrier structures fabricated on deep-level impurity compensated silicon (Si<Ni>, Si<Gd>, Si<Au>, Si<Mn>). The work focuses on elucidating the mechanisms underlying the significant enhancement of pressure sensitivity under pulsed loading compared to static conditions. By constructing a comprehensive theoretical model, we analyze the coupled effects of pressure and induced temperature changes on the electronic properties of the semiconductor bulk and the metal-semiconductor interface. The model quantitatively describes the modulation of the Schottky barrier height due to pressure-induced changes in the semiconductor electron affinity and band gap, alongside the baric and thermal shifts of deep impurity levels in the bulk. It is shown that the dynamic sensitivity arises from the synergistic effect of three primary factors: the baric shift of deep levels (ΔE_i), the pressure-induced change in the barrier height (γP), and the change in base region resistivity (ρ).*

Introduction

The investigation of semiconductor devices under high-pressure conditions is crucial for both fundamental science and applications in sensing and extreme-environment electronics. Schottky barrier diodes, due to their simple structure and sensitivity to surface and bulk properties, serve as excellent probes for studying pressure-induced phenomena. When fabricated on semiconductors containing deep-level impurities—such as transition metals (Ni, Au, Gd, Mn) in silicon—these structures exhibit a complex response to mechanical stress. This complexity arises from the interplay between pressure-induced changes in the semiconductor's bulk electronic properties (carrier concentration, mobility) and the modulation of the metal-semiconductor barrier height itself. While the static piezoresistive effect in bulk semiconductors is well-documented, the dynamic response of Schottky barrier structures under rapid, pulsed hydrostatic pressure remains a less explored frontier. The key scientific gap addressed here is the lack of a unified theoretical model that simultaneously accounts for deep-level ionization kinetics, baric and thermal band structure shifts, dynamic barrier height modulation, and the associated relaxation effects in such structures. This work aims to develop such a model based on provided experimental data, offering a detailed mechanistic understanding of dynamic piezoresistivity in compensated silicon Schottky diodes.

The piezoresistive effect in semiconductors is a classic topic, with established models linking stress to changes in carrier mobility and population via deformation potentials [1]. For semiconductors with deep impurities, the pressure dependence of the ionization energy becomes significant, leading to an enhanced piezoresistive response [2, 3]. Schottky diode current-voltage characteristics are governed by thermionic emission theory, where the barrier height φ_B is a critical parameter sensitive to the semiconductor's electron affinity and band gap [4]. It is known that pressure can alter both these quantities, thereby modulating φ_B [5]. Previous research on pressure effects in Schottky diodes has often focused on homogeneous semiconductors, with less attention given to systems with high concentrations of deep, partially compensated levels. Furthermore, studies under dynamic (pulsed) pressure conditions are scarce. The existing literature highlights phenomena such as long-term persistent photoconductivity and relaxation in disordered systems, often attributed to carrier trapping at metastable defect configurations [6, 7]. However, a coherent theory that integrates the fast, pressure-temperature driven changes in bulk conductivity and barrier height with the subsequent slow relaxation processes specifically for Schottky structures on compensated silicon is missing. This review underscores the need to bridge theories of deep-level pressure coefficients, non-equilibrium thermodynamics, and Schottky barrier electrostatics to explain the observed dynamic sensitivity enhancement.

Theoretical Framework and Modeling

The forward current I in a Schottky barrier diode under zero pressure can be described by thermionic emission theory, considering the voltage drop across the base region with resistivity ρ:

$$I = A^{*}T^{2}\exp\left(-\frac{e\phi_{B0}}{k_{B}T}\right)\left[\exp\left(\frac{e(U-IR_{s})}{nk_{B}T}\right)-1\right] \quad (1)$$

Here, A^{*} is the effective Richardson constant, ϕ_{B0} is the zero-pressure barrier height, U is the applied forward bias, R_s is the series resistance of the quasi-neutral base, n is the ideality factor, and other symbols have their usual meanings. For significant base resistance, $R_s = \rho d/S$, where d is the base thickness and S is the area. Therefore, the voltage across the barrier is $U_b = U - IR_s \approx U - j\rho d$, where j is the current density.

Under applied hydrostatic pressure P, several key parameters become pressure- and temperature-dependent:

1. The deep-level ionization energy in the base: $E_i(P,T) = E_{i0} - \alpha_i P + \beta_i(T - T_0)$.
2. The intrinsic carrier concentration, related to the band gap $E_g(P,T)$.
3. The barrier height: $\phi_B(P,T) = \phi_{B0} - \gamma P + \delta(T - T_0)$, where γ is the pressure coefficient of the barrier height, related to changes in electron affinity and band gap.
4. The base resistivity ρ, which depends on the free carrier concentration n(P,T) and mobility μ(P). For deep-level compensation, $n(P,T) \approx N_d \exp[-(E_{i0} - \alpha_i P)/k_B T]$.

Incorporating these dependencies and assuming the applied pressure induces an adiabatic temperature rise $\Delta T = \eta V_P \Delta P$ (where $V_P = dP/dt$), the current under pressure I_P can be expressed as:

$$I_P = A^*(T_0 + \Delta T)^2 \exp\left(-\frac{e(\phi_{B0} - \gamma P)}{k_B(T_0 + \Delta T)}\right) \exp\left(\frac{e(U - j\rho_P d)}{nk_B(T_0 + \Delta T)}\right) \qquad (2)$$

where ρ_P is the pressure-dependent base resistivity. The relative change in current, which defines the piezosensitivity, is $\Delta I/I = (I_P - I)/I$. From equations (1) and (2), and considering the dominant exponential terms, we derive the expression for the sensitivity coefficient S:

$$S = \frac{\Delta I}{I}\frac{E^o}{P} \approx \frac{E^o}{P}\left[\frac{\phi_{B0} - eU + ejd\rho_P}{\phi_{B0} - eU + ejd\rho_0} \exp\left(\frac{\alpha_i P + \gamma P + ed\Delta\rho/k_B}{k_B(T_0 + \Delta T)}\right) - 1\right] \qquad (3)$$

Here, E^o is Young's modulus used for normalization, and $\Delta\rho = \rho_P - \rho_0$. Equation (3) reveals the three primary physical contributions to the dynamic piezosensitivity encapsulated in the exponential argument:

1. α_i P: The baric shift of the deep impurity level in the base, enhancing carrier generation.

2. γP: The pressure-induced change in the Schottky barrier height, facilitating carrier injection.

3. $ed\Delta\rho/k_B$: The change in the ohmic voltage drop across the base due to altered resistivity.

The analysis of the relative magnitudes of these terms, based on provided experimental parameters $(\alpha_i \sim 10^{-11} eV/Pa, \gamma \sim 10^{-11} eV/Pa, \Delta\rho)$, explains the observed bell-shaped dependence of sensitivity on base resistivity. For a base resistivity around 10^3 Ω·cm, all three terms are comparable, leading to maximal sensitivity. For lower resistivity, the Δρ term is small, and sensitivity is governed by α_i P and γ P (bulk and interface effects). For higher resistivity, the Δρ term dominates, but the overall series resistance limits the current, reducing sensitivity.

The developed theoretical model, which relates carrier concentration to pressure and temperature via equations accounting for deep-level ionization and barrier height modulation, inherently describes a system driven out of equilibrium during a pressure pulse. The return to equilibrium after the rapid removal of the external stress is not instantaneous, as the governing kinetic processes possess finite time constants. The relaxation dynamics can be theoretically derived by considering the system's response to the sudden change in the driving forces. The rapid component of the relaxation is directly linked to the cooling of the semiconductor base after adiabatic heating, a process described by the thermal coupling term η in the relation ΔT = η V_P ΔP. Once the pressure rate V_P becomes zero, the temperature evolves according to a thermal dissipation equation, leading to an exponential decay of the ΔT term in the denominator of the exponential arguments in key equations (such as Eq. 3 in the model). This temperature decay modifies the carrier concentration n(P,T) with a characteristic thermal time constant.

However, a slower relaxation component emerges from the kinetics of the deep-level impurities themselves. The theoretical expression for carrier concentration $n \approx N_d exp[-(E_i 0 - \alpha_i P)/k_B T]$ assumes instantaneous equilibration between the deep level and the conduction band. In reality, the capture and emission rates of carriers by deep levels, especially in a compensated material with a fluctuating potential, are finite. After the rapid ionization event (increase in n), the re-establishment of the equilibrium charge state on the deep levels is governed by a rate equation of the form $dn/dt = -(n - n_{eq})/\tau_{el}$, where n_{eq} is the equilibrium concentration at the final pressure and temperature, and τ_{el} is the characteristic electronic relaxation time. This time constant can be significantly large (seconds to minutes) if the process involves overcoming an energy barrier related to a lattice configurational change around the impurity or carrier percolation in a disordered potential. The full temporal evolution of the current can thus be phenomenologically modeled by a combined solution accounting for both the thermal (τ_{th}) and electronic (τ_{el}) relaxation channels, which explains the multi-stage decay observed in the experimental kinetics

Conclusion. A detailed theoretical model has been developed to explain the dynamic piezoresistive behavior of Schottky barrier diodes fabricated on deep-level impurity compensated silicon. The model successfully integrates the effects of pulsed hydrostatic pressure on both the semiconductor bulk (through baric shifts of deep levels and temperature rise) and the metal-semiconductor interface (through modulation of the barrier height). The derived expression for sensitivity elucidates the competing roles of deep-level ionization, barrier height change, and base resistivity variation, accurately predicting the observed maximum sensitivity for a base resistivity of approximately 10^3 Ω·cm. Furthermore, the model provides a framework for understanding the temporal relaxation of the current following a pressure pulse, attributing it to combined thermal and electronic recovery processes involving deep-level states. These insights are fundamentally important for understanding non-equilibrium carrier dynamics in disordered semiconductor systems under transient stress and are directly applicable to the optimization of high-sensitivity, fast-response pressure sensors based on Schottky diode structures.

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