RELAXATION PHENOMENA AND DYNAMIC PIEZORESISTIVITY IN GOLD-DOPED COMPENSATED SILICON UNDER PULSED HYDROSTATIC PRESSURE

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Abstract: This study presents a comprehensive theoretical and experimental analysis of dynamic piezoresistivity and long-term relaxation phenomena in gold-doped compensated silicon subjected to pulsed hydrostatic pressure. While the electrical properties of Si<Au> have been extensively characterized under static conditions, the complex interplay between deep-level ionization, baric and thermal shifts, and configurational metastability under rapid pressure transients remains inadequately understood. The work is based on provided experimental data detailing current kinetics, carrier concentration, and mobility in Si<Au> samples with varying degrees of compensation. A detailed theoretical model is developed, incorporating the pressure and temperature dependence of deep-level ionization energies, the thermomechanical heating effect, and a two-stage relaxation mechanism involving electronic and configurational processes. The analysis quantitatively separates the contributions of direct baric effects (≈39%) and pressure-stimulated thermal effects (≈61%) to the transient conductivity surge. Furthermore, the observed slow current relaxation (τ ~ minutes) is explained through a model of pressure-induced configurational transitions of gold atoms between interstitial and substitutional sites, with relaxation governed by tunneling and percolation in a strongly compensated, fluctuating potential. These findings provide a fundamental advancement in understanding non-equilibrium carrier dynamics in deep-level systems under impulsive loading and offer critical insights for the design of fast, sensitive piezoresistive sensors with predictable relaxation behavior.

Introduction

The investigation of semiconductor behavior under extreme conditions of pressure and strain is pivotal for both fundamental solid-state physics and advanced device engineering. Deep-level impurities, such as transition metals in silicon, introduce localized electronic states within the bandgap that dramatically alter carrier

recombination, transport, and response to external fields. Gold-doped silicon (Si<Au>) serves as a canonical system due to gold's ability to form stable deep donor and acceptor levels, making it invaluable for controlling carrier lifetime. Although the static piezoresistive effect in silicon and the basic electronic structure of gold centers are well-documented, the response of this complex system to dynamic, non-equilibrium stimuli like pulsed hydrostatic pressure constitutes a significant knowledge gap. Under such conditions, the system experiences concurrent and rapid changes in mechanical stress, lattice temperature, and electric field, driving it far from equilibrium. The specific scientific lacuna addressed herein is the absence of a unified theoretical framework that can explain the complete temporal response—including the immediate dynamic piezoconductivity and the subsequent protracted relaxation—observed in compensated Si<Au>. This work aims to construct such a framework through a meticulous analysis of provided experimental data, focusing on the roles of deep-level ionization kinetics, baric and thermal shifts, and impurity configurational metastability.

Gold in silicon has been the subject of decades of research, establishing its nature as an amphoteric impurity introducing two primary deep levels: an acceptor level approximately 0.54 eV below the conduction band edge ($E_c - 0.54eV$) and a donor level about 0.36 eV above the valence band edge ($E_v + 0.36eV$) [1, 2]. These levels exhibit significant pressure coefficients, unlike shallow impurities, due to their strong localization and interaction with the lattice deformation potential [3]. It is also established that gold can exist in multiple charge states (Au^+, Au^0, Au^-), and theoretical models suggest the total energy of a gold center depends on its specific lattice configuration—whether it resides in a substitutional site (Au_s) or is displaced into an interstitial position (Au_i) [4]. Research on persistent photoconductivity and long-term relaxation in compensated semiconductors has often attributed these phenomena to the spatial inhomogeneity of the potential landscape and slow emission/capture kinetics via deep levels [5, 6]. However, previous studies have predominantly examined these effects under optical or thermal excitation in the absence of significant mechanical stress. The unique aspect of pulsed pressure loading is the simultaneous induction of band structure deformation, Joule or deformation heating, and possible atomic rearrangements. While some works have touched upon dynamic piezoresistance [7], a holistic model that integrates the instantaneous pressure-temperature-conductivity relationship with the subsequent slow, configurational relaxation specific to Si<Au> has not been proposed. This review highlights the necessity to bridge the understanding of electronic deep-level physics with lattice dynamics and kinetic theory to fully describe the observed phenomena.

Theoretical Framework and Modeling

The core of the proposed model rests on describing the non-equilibrium carrier concentration in a semiconductor containing a dominant deep impurity level under

time-varying pressure P(t) and temperature T(t). The starting point is the expression for the electron concentration emanating from a deep donor level with ionization energy E_i under equilibrium conditions:

$$n(P,T) = N_d \exp\left(-\frac{E_i(P,T)}{k_B T}\right) \quad (1)$$

Here, N_d is the effective density of states, and k_B is Boltzmann's constant. The critical step is to define the pressure and temperature dependence of the ionization energy E_i. It is expressed as a sum of its zero-pressure value at a reference temperature, a linear baric shift, and a thermal contribution often described by Varshni's formula. For the pressure range considered, the linear approximation is sufficient:

$$E_i(P,T) = E_{i0} - \alpha_i P + \beta_i (T - T_0) \quad (2)$$

In this equation, α_i is the baric coefficient (units: eV/Pa), representing the shift of the energy level per unit pressure, and β_i is its temperature coefficient. Substituting Equation (2) into Equation (1) yields the dynamic carrier concentration:

$$n(P,T) = N_d \exp\left(-\frac{E_{i0} - \alpha_i P + \beta_i (T - T_0)}{k_B T}\right) \quad (3)$$

For the transient regime during and immediately after a pressure pulse, the temperature is not independent but is coupled to the pressure via the thermomechanical effect, approximated as $T(P) = T_0 + \eta P(t)$, where η is a heating coefficient dependent on the material and pulse characteristics. Introducing this into Equation (3) gives a coupled expression:

$$n(P) = N_d \exp\left(-\frac{E_{i0} - \alpha_i P + \beta_i \eta P}{k_B (T_0 + \eta P)}\right) \quad (4)$$

The relative change in concentration, which is proportional to the relative change in conductivity given the experimentally observed minor variations in carrier mobility, is::

$$\frac{n(P)}{n_0} = \exp\left(\frac{E_{i0}}{k_B T_0} - \frac{E_{i0} - (\alpha_i - \beta_i \eta) P}{k_B (T_0 + \eta P)}\right) \quad (5)$$

where $n_0 = n(0, T_0)$. To separate the "pure" baric effect from the thermal effect, we consider two hypothetical scenarios. First, an isothermal pressure application (dT=0):

$$\left(\frac{n(P)}{n_0}\right)_{\text{baric}} = \exp\left(\frac{\alpha_i P}{k_B T_0}\right) \quad (6)$$

Second, a purely thermal excitation at zero pressure that leads to the same final temperature $T = T_0 + \eta P$:

$$\left(\frac{n(T)}{n_0}\right)_{\text{thermal}} = \exp\left(\frac{E_{i0}}{k_B T_0} - \frac{E_{i0}}{k_B (T_0 + \eta P)}\right) \quad (7)$$

For small arguments, the exponential can be linearized. Using the experimental parameters from the provided data ($E_i \approx 0.54 eV, \alpha_i \approx 1.81 \times 10^{-11} eV/Pa, \eta P \approx 10 K$ for
$P = 6 \times 10^8 Pa, T_0 = 293 K$), the numerical evaluation of the full expression (5) and

its decomposition shows that the thermal contribution (Equation 7) accounts for approximately 61% of the total concentration increase, while the direct baric term (Equation 6) accounts for about 39%. This quantifies the dominant role of pressure-induced heating in the dynamic sensitivity, explaining why the dynamic piezoresistivity vastly exceeds the static one.

The model must now address the long-term relaxation shown in Figures 4.10 and 4.12, where the current decays over minutes after pressure release, despite the immediate reversal of the baric and thermal drives. This necessitates introducing a slow, metastable process. The proposed mechanism involves a pressure-induced change in the stable lattice configuration of the gold impurity. Let the two relevant configurations be the substitutional gold atom (Au_s) and the gold atom in an interstitial position adjacent to a vacancy ([V-Au_i]). Their respective total energies, U_s(P) and U_i(P), are functions of pressure. Under ambient conditions, [V-Au_i] may be the lower energy state. Under sufficient compressive pressure, the energy minimum may shift, making Au_s more stable. This can be represented by a configurational coordinate diagram. The applied pressure P modifies the potential landscape, reducing the energy barrier for the transition [V-Au_i] → Au_s. This transition is assumed to be fast under high pressure, altering the electronic signature of the gold center and contributing to the conductivity increase. When pressure is released, the Au_s configuration becomes metastable, as the original potential landscape is restored. The system then relaxes back to the [V-Au_i] state via a thermally assisted tunneling process. The relaxation time for such a process is given by:

$$\tau_{rel} = \nu_0^{-1} \exp\left(\frac{\Delta U}{k_B T}\right) \cdot [F_{FC}]^{-1} \qquad (8)$$

Here, ν_0 is an attempt frequency, ΔU is the energy barrier height after pressure release, and F_{FC} is the Franck-Condon factor, which accounts for the overlap of vibrational wavefunctions in the two configurational states and is typically <<1 for deep centers involving large lattice relaxation. Estimates using typical values ($\nu_0 \sim 10^{13} s^{-1}, \Delta U \sim 0.1 - 0.2 eV$, a small F_{FC}) yield τ_rel in the range of tens of seconds to minutes, consistent with the observed kinetics. This configurational relaxation slowly restores the original electronic spectrum of the gold impurities, gradually reducing the carrier concentration back to its baseline. In highly compensated samples, the relaxation is further slowed by the need for carriers to percolate through a disordered potential landscape, adding another time-dependent factor to the conductivity decay.

Results and Discussion

The key experimental results are the immediate jump in current synchronous with the pressure pulse and the temperature increase (ΔT ≈ 8-11 K), followed by a slow decay of current over minutes after pressure release, **as recorded in the kinetic**

measurements of current versus time. Hall effect measurements conclusively show that the current change is predominantly due to a change in carrier concentration n, with mobility μ remaining largely constant. The magnitude of the initial current peak is strongly dependent on the sample's resistivity (degree of compensation), with higher resistivity samples showing larger peaks. The developed theoretical model successfully explains these observations. The immediate response is modeled by Equations (4) and (5), capturing the synergy between baric level shift and thermal ionization. The quantitative 39%/61% separation aligns with the observed correlation between current and temperature transients. The slow relaxation is not captured by these instantaneous equations and is instead attributed to the configurational metastability mechanism described by Equation (8). The dependence on the degree of compensation supports the involvement of a percolative process in the relaxation phase. The proposed two-stage model—fast electronic excitation followed by slow configurational relaxation—provides a coherent and quantitative explanation for the full temporal evolution of conductivity in Si<Au> under pulsed pressure.

Conclusion

This work presents an advanced theoretical model that elucidates the complex dynamic piezoresistive response and subsequent relaxation in gold-doped compensated silicon under pulsed hydrostatic pressure. The model rigorously decomposes the transient conductivity surge into a direct baric component (≈39%) and a dominant pressure-induced thermal component (≈61%), providing a quantitative explanation for the enhanced dynamic sensitivity. Furthermore, it introduces a novel explanation for the observed long-term relaxation by invoking a pressure-triggered, metastable configurational change of gold impurities, with relaxation kinetics governed by a thermally assisted tunneling process. This framework successfully integrates deep-level ionization theory, lattice dynamics, and kinetic models of configurational transitions. The findings significantly deepen the understanding of non-equilibrium processes in semiconductors with deep impurities and provide essential guidelines for the development of piezoresistive sensors where speed, sensitivity, and post-stimulus recovery are critical design parameters.

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