Graphical Representation and Origin of Piezoresistance Effect in Germanium

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Abstract. The longitudinal and transverse piezoresistance coefficients of Ge at room temperature are represented graphically as a function of the crystal directions for orientation (001), (110) and (211) planes. Many valley model of conduction band and stress decoupling decoupling of the degenerate valence band into two bands of prolate and oblate ellipsoidal energy surface are shown to explain origin of the piezoresistance. One this basis, comparison between piezoresistance coefficient and theoretical model is discussed.

1. Introduction

Sixty years has passed since Smith [1] reported the piezoresistance (PR) effect, and Dresselhaus, Kip and Kittel (D-K-K) investigated the cyclotron resonance of electrons and holes, in Ge and Si crystals [2]. Origin of the PR effect in n-type Si was explained by carrier redistribution between the many valleys and the deformation of the valleys [3]-[5]. The PR of p-type Si has been also reported by several researchers [6]-[10].

Recently, Ge has been used in the framework of heterostructure microelectronics and high speed RF devices. However, in spite of the growing utility of Ge in these devices, and in spite of many studies for strained Si, origin of PR property of Ge as the counterpart of Si has not been fully given since the pioneering work of Smith and D-K-K.

In the present paper, typical PR coefficients of Ge are represented graphically as a functions of crystal orientations. By analogy to the theory for Si, origin of PR in Ge is explored theoretically. Correlations between the hole effective masses and the longitudinal and transverse PR coefficients of p-type Ge are discussed. The presented results should be of value for researchers to design heterostructure devices.

2. Dependence on Crystallographic Axis

According to the phenomenological description, the fractional change in resistivity with small stress is expressed with the PR coefficients;

\[
\frac{\Delta \rho_i}{\rho} = -\frac{\Delta \sigma_i}{\sigma} = \sum_{j=1}^{6} \pi_{ij} X_j
\]  

(1)
where $X_j$ is the component of the stress tensor in six-component vector notation and $\pi_{ij}$ is the component of the PR tensor. In crystals with cubic symmetry such as silicon and germanium, independent components of the PR tensor are $\pi_{11}$, $\pi_{12}$ and $\pi_{44}$.

The transformation is given by direction cosines. Here, three typical PR coefficients will be considered. The first one is a longitudinal PR coefficient when current and field are in direction of the uniaxial stress noted by $\pi_l$. The second one is the transverse PR coefficient when the current and field are perpendicular to the stress noted by $\pi_t$. And the third one is the shear PR coefficient $\pi_s$.

$$\pi_{11}' = \pi_l = \pi_{11} - 2(\pi_{11} - \pi_{12} - \pi_{44})(l^2 m^2 + m^2 n^2 + n^2 l^2)$$
$$\pi_{12}' = \pi_t = \pi_{12} + 2(\pi_{11} - \pi_{12} - \pi_{44})(l^2 l^2 + m^2 m^2 + n^2 n^2)$$
$$\pi_{66}' = \pi_s = \pi_{44} + 2(\pi_{11} - \pi_{12} - \pi_{44})[(l_1 l_2)^2 + (m_1 m_2)^2 + (n_1 n_2)^2]$$

In an $(lmn)$ plane, the graph can be obtained by making the axis $3'$ normal to the plane, that is, $[l_3 m_3 n_3] = (l + m + n)^{1/2}[lmn]$

The graphs of room temperature as a function of crystal direction for orientations in the $(001)$, $(011)$, and $(211)$ planes are shown in Fig. 1 and 2. The graphs are shown based on the data of Smith. The upper halves of the graphs show positive values of the PR coefficients, that is the resistance increases with tensile stresses. The lower halves in the figures show negative values of the PR coefficients, that is, the resistive decreases with tensile stresses.
3. Origin of Piezoresistance Effect

3.1. Many-Valley Model
According to Herring and Vogt [4], the energy surfaces at the band edges are ellipsoid and the carriers transfer between band edges which are shifted individually by stress. Assuming that mobilities (\( \mu^{(i)} \)) are independent of stress, the change in conductivity under stress is given by

\[
\Delta \sigma = n e \left( -\frac{1}{kT} \right) \sum_{i=1}^{V} \mu^{(i)} \left( \Delta E^{(i)} - \frac{1}{V} \sum_{j=1}^{V} \Delta E^{(j)} \right)
\]

where \( V \) is the total number of valleys and \( \Delta E^{(i)} \) is the energy shift at the \( i \)-th ellipsoid band-edge [3].

3.2. Conduction Band
The band-edge shift of each valley in C.B. are given by the deformation potential analysis (Table 1) [3]. Since all band edges in C.B. of Ge shift in same way under \( \langle 100 \rangle \) stress, conductivity does not change, that is \( \pi_{11} \) and \( \pi_{12} \) vanish. Then we consider the change in conductivity under \( \langle 111 \rangle \) stress. Conversion of the mobility tensor of each valley gives its components for \( \langle 111 \rangle \), \( \langle 1 \overline{1} 0 \rangle \) and \( \langle 1 \overline{1} 2 \rangle \) directions (Table 1).

Table 1 Components of mobility and band edge energy shift for valleys, where \( \Delta = s_{11} + 2s_{12} \), \( \Xi_d + \Xi_u/3 \) and \( \Xi_u \) are the deformation potentials for dilation and pure shear, respectively.

| Mobility Valley | \( \mu^{(i)}_{\langle 111 \rangle} \) | \( \mu^{(i)}_{\langle 11 \overline{1} \rangle} \) | \( \mu^{(i)}_{\langle 1 \overline{1} 2 \rangle} \) | Band edge shift \( \Delta E^{(i)} \) |
|-----------------|-----------------|-----------------|-----------------|--------------------------|
| \( L_1 \langle 111 \rangle \) | \( \mu \) | \( \mu \) | \( \mu \) | \( (\Xi_d + \Xi_u/3)\Delta \cdot X \pm \Xi_u s_{44} X/3 \) |
| \( L_1 \langle 1 \overline{1} 1 \rangle \) | \( (\mu + 8\mu_{\perp})/9 \) | \( (2\mu + 7\mu_{\perp})/9 \) | \( (4\mu + 7\mu_{\perp})/9 \) | \( (\Xi_d + \Xi_u/3)\Delta \cdot X \mp \Xi_u s_{44} X/9 \) |
| \( L_1 \langle 1 \overline{1} 2 \rangle \) | \( (\mu + 8\mu_{\perp})/9 \) | \( (2\mu + 7\mu_{\perp})/9 \) | \( (4\mu + 7\mu_{\perp})/9 \) | \( (\Xi_d + \Xi_u/3)\Delta \cdot X \mp \Xi_u s_{44} X/9 \) |

Substituting Eq.(3) for the Eqns. in Table 1 and using Eqns. (1) and (2), the expression of \( \pi_{44} \) of n-Ge can be obtained as,

\[
\pi_{11} = 0, \quad \pi_{12} = 0, \quad \pi_{44} = -\frac{K - 1}{2K + 1} \frac{\Xi_u s_{44}}{3kT}
\]

where \( K = \mu_{\perp} / \mu_{\parallel} \equiv m_{\perp} / m_{\parallel} \) is the mobility anisotropy factor of conduction band edge.

3.3. Valence Band
By an analogy to many-valley theory, we can consider the hole transfer between the two bands (i.e. the heavy hole band and the light hole band) which are decoupled by the stress application. The energy surfaces of the two bands under a uniaxial stress are prolate and oblate ellipsoidal (Table 2) [8][9].

Since the density-of-state effective masses for HH and LH are compatible under stress, the change of conductivity of Eq.(3) can be written as,

\[
\Delta \sigma \equiv n e \left( \mu^{(HH)} - \mu^{(LH)} \right) \cdot \frac{\Delta E}{2kT}
\]

where \( \mu = e^2 \tau/m \). It is noteworthy that the change of conductivity is proportional to the difference between HH and LH mass values [10][11]. Substituting Eq.(1) for above equation and Eqns. in Table 2, the PR coefficients of p-Ge can be expressed as,
\[ \pi_{11} = \frac{B}{A} \cdot \frac{b(s_{11} - s_{12})}{kT}, \quad \pi_{12} = -\frac{B}{2A} \cdot \frac{b(s_{11} - s_{12})}{kT}, \quad \pi_{44} = \frac{N}{3A} \cdot \frac{ds_{44}}{2\sqrt{3}kT} \]

where \( N/3 = \sqrt{B^2 + C^2/3} \).

Table 2. Longitudinal and transverse inverse masses of two bands under \( \{100\} \) and \( \{111\} \) stress, and band-edge shift of V.B., where \( A, B \) and \( N \) are inverse mass parameters, \( b \) and \( d \) are the deformation potentials, and upper and lower signs denote the light and the heavy hole bands, respectively.

| Inverse mass of ellipsoidal energy surface | Band edges shift \( \Delta E \) |
|------------------------------------------|-------------------------------|
| \( \{100\} \) stress | \( \{111\} \) stress |
| \( A \pm B \) | \( A \mp B/2 \) | \( A \pm N/3 \) | \( A \mp N/6 \) | \( b(s_{11} - s_{12})X \) | \( \frac{1}{2\sqrt{3}} ds_{44}X \) |

4. Discussions

In a quantitative argument, the following data are used: \( A = -13.1 \), \( B = 8.3 \), \( C = 12.5 \), \( \Xi_u = 18.7 \), \( b = 2.1 \) eV, \( K = 19.3 \) and \( s_{11} = 0.964 \), \( s_{12} = -0.260 \), \( s_{44} = 1.49 \times 10^{-12} \text{ cm}^2/\text{dyne} \) [7]. The PR coefficients calculated by the many valley model are summarized in Table 3 as a comparison with the experimental data [1].

Table 3. Theoretical and experimental PR coefficients of Ge at 300 K \( (\times 10^{-12}\text{ cm}^2/\text{dyne}) \). The figures in parentheses indicate the values estimated by high temperature approximation.

| n-Ge | p-Ge |
|------|------|
| \( \pi_{11} \) | \( \pi_{12} \) | \( \pi_{44} \) | \( \pi_{11} \) | \( \pi_{12} \) | \( \pi_{44} \) |
| Theory | 0 | 0 | -165 | 62.7(-0) | -31.3(-0) | 148(-97) |
| Experiment | -2.3 | -3.2 | -138 | -3.7 | 3.2 | 96.7 |

Agreement between the theoretical and the experimental values is good but for the unusually large \( \pi_{11} \) and \( \pi_{12} \) of p-Ge. One of the reasons for the discrepancies is due to the low temperature approximation (\( \Delta E > 2kT \)). Since the magnitude relation of the transverse mass values of two bands is reversed at low temperature [11], the difference between them should be smaller at a high temperature. If the assumption on the DOS effective masses is incorrect in high temperature region, the magnitude of band parameters “B” and “N” in Eq. (6) will decrease, and \( \pi_{11} \), \( \pi_{12} \) and \( \pi_{44} \) will become close to the experimental values. The discrepancy of \( \pi_{11} \) and \( \pi_{12} \) in n-Ge should be attributed to the destruction of the rotational symmetry of the ellipsoidal valleys by stress [12].

References

[1] Smith C S 1954 Phys. Rev. 94 42
[2] Dresselhous G, Kip F and Kittel C 1955 Phys. Rev. 98 368
[3] Kanda Y 1982 IEEE Transaction on Electron Devices ED-29(1) 64
[4] Herring C and Vogt E 1956 Phys. Rev. 101 944
[5] Matsuda K, Suzuki K, Yamamura K and Kanda Y 1993 J. Appl. Phys. 73(4) 1838
[6] Pikus G E and Bir G L 1960 Soviet Physics –Solid State 1 1502
[7] Kanda Y 1987 Jpn. J. Appl. Phys. 26(7) 1031
[8] Hensel J C and Feher G 1963 Phys. Rev. 129(3) 1041
[9] Suzuki K, Hasegawa H and Kanda Y 1984 Jpn. J. Appl. Phys. 23(11) L871
[10] Kanda Y and Matsuda K 2004 Proceedings of the 27th ICPS (Arizona USA) 79
[11] Matsuda K 2004 Journal of Computational Electronics 3 273
[12] Kanda Y and Suzuki K 1991 Phys. Rev. B 43(8) 6754