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Uniaxial Stress DLTS of Iron-Acceptor Pairs in Silicon

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Abstract

Deep Level Transient Spectroscopy (DLTS) under uniaxial stress has been applied to the FeB level at E_V + 100 meV in silicon, and to both the FeAl(2) and FeAl(1) levels in silicon at E_V + 130 meV and E_V + 200 meV respectively. No splittings of the DLTS peaks were observed, however large, anisotropic shifts in the peak temperatures occured. We modeled thermal emission to a stress-split valence band to fit the defect energy under uniaxial compression. Although these defects exhibit axial symmetry in EPR, the stress anisotropy suggests that at the elevated temperatures of DLTS the defects freely reorient under applied stress according to T_2 symmetry of the tetrahedral group.

I. Introduction

Iron-Acceptor pairs in silicon exhibit a variety of symmetries when observed by electron paramagnetic resonance (EPR) and photoluminescence (PL). A single trigonal defect has been observed in Si:FeB using EPR [1, 2, 3], while both a trigonal and a rhombic I defect have been observed in Si:FeAl[3]. In addition, FeGa is observed to have trigonal symmetry in EPR, but FeIn exhibits rhombic I symmetry [1 , 3]. In photoluminescence rhombic I and trigonal symmetry have been observed for FeIn and FeTl [4]. The photoluminescence of FeB, on the other hand, showed no axial symmetry under the application of a magnetic field which led the authors to suggest that the FeB defect observed in PL was not the same as the defect observed in EPR[5].

Several of these defects produce energy levels deep in the band gap which can be seen by deep level transient spectroscopy (DLTS). A single defect is observed in Si:FeB, which was therefore assumed to be the same as the single trigonal center seen in EPR. Corresponding to the two FeAl defects observed in EPR, there are two defects related to FeAl seen in DLTS: FeAl(1) at E_V + 0.2 eV, and FeAl(2) at E_V + 0.13 eV. Chantre et. al. [6] have demonstrated that the FeAl(2) level is a metastable state of the FeAl(1) defect. They further postulated that the

FeAl(2) defect corresponds to the rhombic EPR center, while FeAl(1) corresponds to the trigonal EPR center, similar to the FeB defect.

We have applied uniaxial stress in conjunction with DLTS to investigate the symmetry properties of the iron-acceptor defects observed in DLTS and to understand the different symmetries which are observed using various techniques.

II. Data and Analysis

Iron was diffused into B and Al doped silicon at 1000 °C for 2 to 4 hours either from random sources or from a coating of ferric chloride. Oriented samples were cut into parallelepipeds with 1 mm^2 cross sections and lengths ranging from 3.5 mm to 6 mm. The Shottky contacts were made by evaporating Al onto the middle third of the sample. Gold was used for the ohmic contact. The stress data were taken by setting the correlator time constant to a fixed value and increasing the stress by increments of about 0.1 GPa up to nearly 1 GPa. The data were always taken for increasing temperature under 1/10 atm of He. Figure 1 shows typical stress data for FeB stressed along <110>. The correlator time constant was set at 4 ms. Two features are immediately apparent: there is no noticible broadening of the DLTS peak; and there is a substantial shift in the peak to lower temperatures. The lack of significant broadening removes the possibility of splitting greater than about 3 meV/GPa. Part of the shift in temperature of the

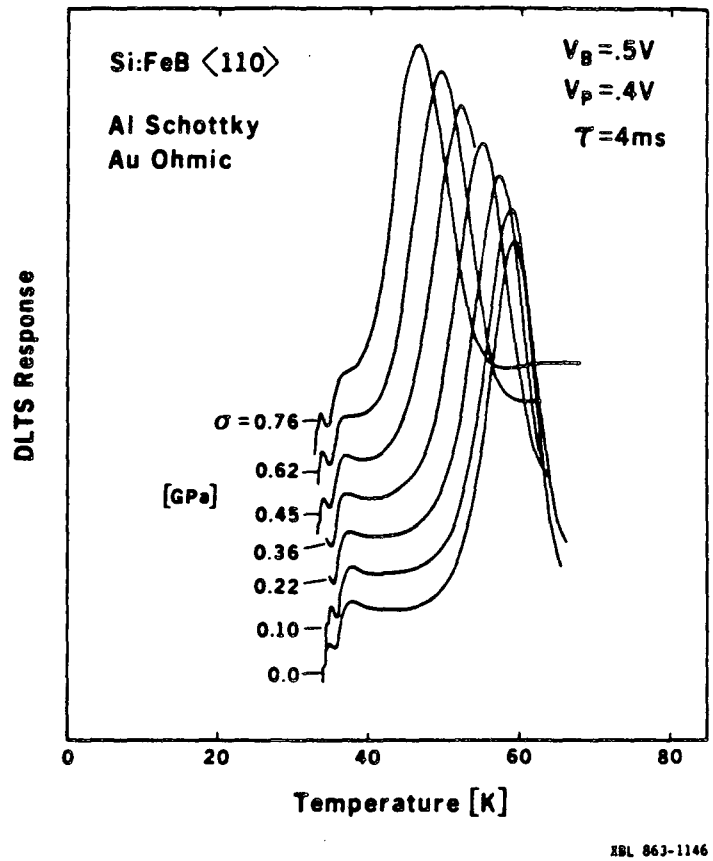

figure 1. Shift of DLTS peak under <110> stress for constant emission rate.

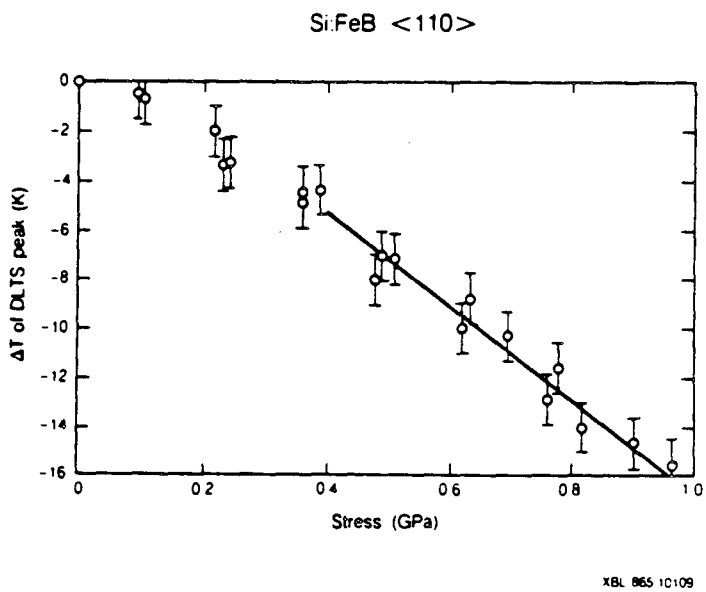

figure 2. Data for shift of DLTS peak under <110> stress. Solid line is fit to the defect energy shift.

peak can be explained in terms of thermal emission to a stress-split valence band.

Application of uniaxial stress splits the Γ_8 degenerate valence band into a light-hole band and a heavy-hole band. The thermal emission of carriers from a defect level to these bands are independent, competing process. Therefore the individual probabilities add to give a single transition probability. This probability is

$$e_0(\tau) = c\,T^2 \{ \sigma_L(\tau)\, m^*_L(\tau) \exp[-(E_T(\tau) - E_L(\tau))/kT] + \sigma_H(\tau)\, m^*_H(\tau) \exp[-(E_T(\tau) - E_H(\tau))/kT] \} \qquad (1)$$

where H and L refer to the heavy and light hole bands, $\sigma(\tau)$ are the capture cross sections, $m^*(\tau)$ are the effective masses, $E_T(\tau)$ is the trap energy, and $E(\tau)$ are the band edge energies.

The single transition rate e_0 produces a single exponential transient, and therefore a single DLTS peak shifted in temperature as a function of τ. It is interesting to note, however, that the Arrhenius plot is non-linear in temperature. Defect degeneracies are also split by uniaxial stress, and these can give rise to single or multiple peaks, depending on the relation between repopulation (or reorientation) rates and thermal emission rates.

The energy shift of the defect as a function of stress can be fit using equation 1. In general, all of the parameters can vary as a function of stress. The analysis is simplified by only fitting the stress data in the regime of stresses greater than 0.4 GPa. Above this value of stress the effective masses saturate to constant values[7], and the effects from the higher states of a split ground state manifold are reduced. Typical data for <110> stress of FeB is shown in figure 2 along with the theoretical fit from equation 1. The defect energy is the only adjustable parameter.

This analysis was carried out for <100>, <110>, and <111> stress for FeB, FeAl(1), and FeAl(2). The results for FeB are plotted in figure 3 for one GPa stress. The splitting of the valence band is also included in the figure. After the hydrostatic contribution to the defect energy [8] is subtracted away, a large shear anisotropy remains. The results for both FeAl defects are plotted in figure 4. FeAl(1) has nearly identical shear anisotropy as FeB. The hydrostatic shift of the metastable state, FeAl(2), has not been measured, so quantitative statements cannot

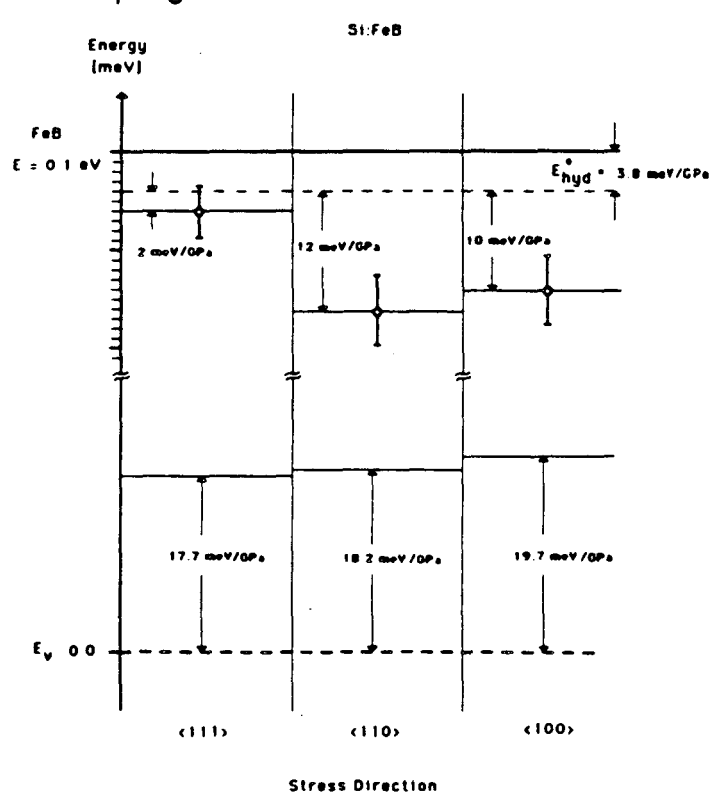

figure 3. Energy shifts for FeB under 1 GPa stress. Splitting of the valence band is included.

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be made concerning the shear anisotropy of this defect. However, if the hydrostatic contribution to the energy shift is comparable to the hydrostatic shifts of the other defects, then FeAl(2) has qualitatively the same stress dependence as FeB and FeAl(1).

The stress anisotropy of FeB and FeAl(1) corresponds closely to the lowest energy configuration of a defect with either rhombic I symmetry or with T_2 symmetry of the tetrahedral group. The splittings of a T_2 state and a rhombic I state , fit to the data of FeB, are shown in figure 5 and figure 6 respectively. Because the iron-acceptor pairs are certainly axial defects, this data by itself would suggest that the stable DLTS defects are the rhombic I defects observed by EPR and PL, and that the trigonal defects are either not observed, or are metastable. Yet the stress behavior of FeAl(2), shown in figure 4, is entirely inconsistent with trigonal symmetry, and in fact closely resembles the stress dependence of FeB and FeAl(1). This would indicate that there is a high multiplicity of rhombic defects observed by DLTS, with no trigonal centers. In other words, the symmetries of the predominant defects observed in DLTS would not correspond to the symmetries of the predominant defects observed by EPR in the same samples, and the list of iron-acceptor pair symmetries mentioned in the introduction to this article would become even longer.

These difficulties can be resolved if all the iron-acceptor defects indeed have T_2 symmetry. This would be plausible if the defects could be represented essentially as simple electric dipoles. A dipole centered at a site of tetrahedral symmetry has T_2 symmetry and has the same total energy for any orientation. Such an isotropic defect would be free to orient in the crystal unhindered by potential barriers, although it would exhibit stress anisotropy characteristic of T_2 symmetry as the crystal symmetry is lowered. Small local energy minima might still exist in the <111> and <100> directions, which would explain the variety of symmetries observed at low temperature by EPR and PL. But these minima would be overwhelmed by the anisotropic strain field, and at the relatively high temperatures of DLTS the iron could freely orient in any direction in the plane perpendicular to the stress direction. The dipoles oriented perpendicular to the stress direction have lower total energy than those oriented parallel to the stress for both compression and tension. Although the dipole configuration has T_2 symmetry, the symmetry of the electron in

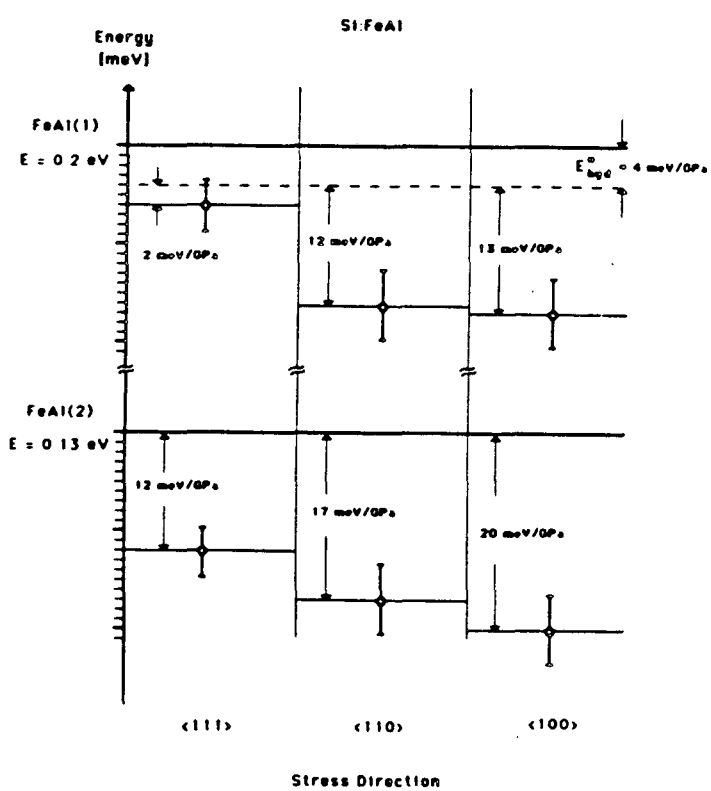

figure 4. Energy shifts for both FeAl defects.

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the iron d-shell has a much lower symmetry relevant to the instantaneous orientation of the defect in the crystal, and in general is an orbital singlet. The observed stress anisotropy of the electronic state is only a reflection of the rearrangement of the dipole under stress.

Despite the fact that figure 5 and figure 6 look qualitatively similar, they describe entirely different phenomena. The splittings for rhombic I symmetry arise from the fact that the iron is constrained to lie in <100> directions. The splittings for configurational T_2 symmetry, on the other hand, merely describe the energy surface for the defect which can still essentially orient in any direction in the crystal. Such freedom of movement is inconsistent with the models from EPR in which the iron is situated in nearest-neighbor and next nearest-neighbor interstitial sites in relation to the acceptor. Rather, the iron must be situated extremely closely to the substitutional site. In fact FeAl(2) must differ from FeAl(1) by some structural rearrangement [6], either nuclear or electronic, but the iron must remain sufficiently close to the substitutional site to allow free orientation in the crystal. Based on our experimental error, however, we cannot rule out the possibility that the FeB and FeAl(1) have configurational T_2 symmetry with slight trigonal distortions, while FeAl(2) indeed has rhombic I symmetry.

III. Conclusion

The great variety of symmetries observed for iron-acceptor pairs using different techniques at different temperatures can be reconciled by assuming that the defects are essentially isotropic dipoles with configurational T_2 symmetry. Localized energy minima may occur in the <111> and <100> directions, but these must be small and easily overwhelmed by thermal motion and strain fields.

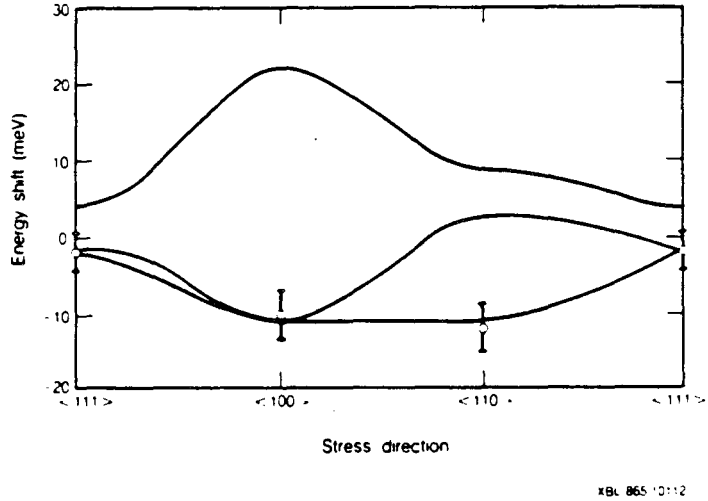

figure 5. Energy shifts of a T_2 state for 1 GPa stress [9].

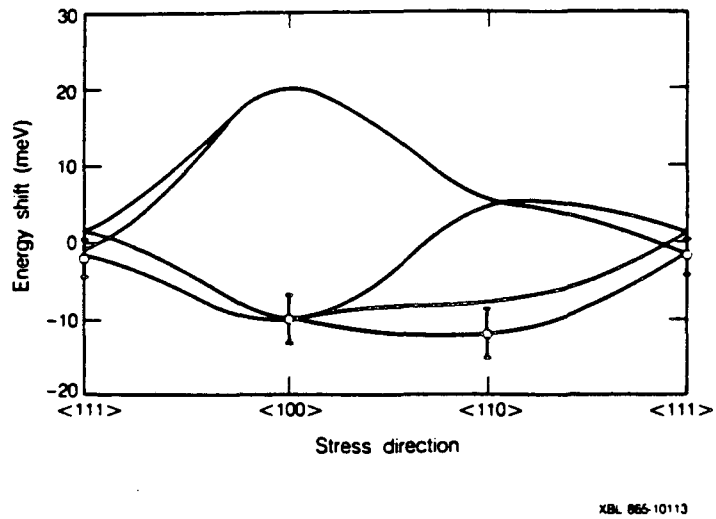

figure 6. Energy shifts of a rhombic I defect for 1 GPa stress [10].

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