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EXCHANGE-CORRELATION EFFECTS IN SILICON INVERSION LAYERS: VALLEY OCCUPANCY PHASE TRANSITIONS

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Exchange-correlation effects can lead to spontaneous symmetry breaking in many valley systems. This idea is applied to valley occupancy phase transitions in silicon inversion layers.

The exchange energy of a degenerate electron gas favors ferromagnetic alignment of the electron spins, while the kinetic and correlation energies favor paramagnetic alignment. Because each of these contributions to the total energy has a different dependence on electron density, it is possible to have a region of density in which the exchange energy dominates and the ferromagnetic state is stable. In semiconductors, equivalent valleys of a many-valley band structure play a role quite analogous to spin. Electrons in different valleys can interact, but they cannot effectively undergo intervalley exchange because the Coulomb interaction is negligibly small at the large momentum transfer required for such a process. Bloss et al. [1] have used this analogy in their recent investigation of the possible two valley to one valley transition on a Si (100) inversion layer. They use a "valley density" functional analogue of the spin density functional [2] to calculate the ground state energies of the one and two valley states. A transition from two valley to one valley occupancy occurs for a density of the order of $2\text{-}3 \times 10^{11}$ cm^{-2}.

The usual density functional approach to correlation effects gives an accurate description of the ground state, but does not adequately describe excited states. Kalia et al. [3] have recently suggested a method of including correlation effects which overcomes this difficulty. They introduce an exchange-correlation potential $V_{xc}\{n(z)\}$ which contains a number of adjustable parameters. The eigenfunctions and eigenvalues of the single particle Hamiltonian (which includes V_{xc}) are determined. Then, the difference, H^1, between the full electron-electron interaction and the single particle approximation (V_{xc}) to it is treated as a perturbation. The adjustable parameters in V_{xc} are chosen in such a way that H^1 has minimum effect on the energy of a particle at the Fermi surface (i.e. the self-energy of such a particle due to H^1 must vanish). Thus V_{xc} still gives an excellent description of the ground state; however the self-energies of excited subbands can now be evaluated so that the excited states can be treated accurately.

This method has been applied to the evaluation of the energy separation E_{10} between the ground and first excited subbands of a Si (100) inversion layer for both two and one valley occupancy [4]. The separation is always larger for single valley occupancy because the exchange energy of the ground subband is larger in magnitude for single valley occupancy. Thus, a $2 \rightarrow 1$ valley occupancy transition

should be revealed as an abrupt change in the position of the E transition energy as the density is lowered through some critical value n_c.

Far infrared Fourier transform spectroscopy [5] has been used to study the intersubband transitions of (100) Si inversion layers. Some experimental results for the subband transition energies are shown in Fig. (1). Figure (1a) shows the $0 \rightarrow 1$ transition energies for a (100) MOSFET with a peak mobility of 8000 $cm^2/V\text{-sec}$. The experimental points fit the calculation of Ando [6] for an appropriate depletion charge extremely well over the entire range of carrier density. There is no measurable shift in E_{10} away from the theoretical curve down to the lowest density measurable. Figure (1b) shows the subband transition energies for a sample with a peak mobility of 11,000 cm /V-sec. This sample is actually tilted 1.2° away from the (100) direction, but this should not affect its behavior at the densities of interest. For this sample there is a marked change in slope of the transition energy (both $0 \rightarrow 1$ and $0 \rightarrow 2$) as a function of carrier density at about $5 \times 10^{11} cm^{-2}$. This is somewhat higher than the critical density predicted by Bloss et al. [1]. At densities below this value, the transition energies are shifted $\lesssim 1$ meV higher in energy than would be expected from Ando's result for two valley occupancy. This shift is somewhat larger than that calculated by Kalia and Quinn [4] for two valley $\rightarrow$ one valley occupancy but qualitative features are as expected for this transition. It is likely that a similar transition is not observed in the lower mobility sample due to localization which sets in at $5 \times 10^{11} cm^{-2}$ in that sample (see Fig. (1)).

These ideas have also been applied to the sixfold degenerate Si (111) inversion layer. A many body calculation of the ground state energy which allows for unequal valley occupancy has been carried out using a local "valley density" functional. The exchange-correlation potential of a v-valley system is determined from the results for a one valley degenerate electron gas by the scaling relation $E_{xc}^{(v)}(n_s) = v\, E_{xc}^{(1)}(v^{4/3} n_s)$, where $E_{xc}^{(v)}(n_s)$ is the exchange-correlation energy per particle for a v-valley system with density $n=(3/4\pi)(a^*r_s)^{-3}$. $a_o^*=t\,\varepsilon_s/m^*e$ is the effective Bohr radius ($\sim 1.6 \times 10^{-7} cm$ for (111)-Si), m* the optical effective mass, and ε_s the dielectric constant of Si. This scaling relation is exact in both the RPA and plasmon pole approximation [7]. The energy per particle of the six valley and

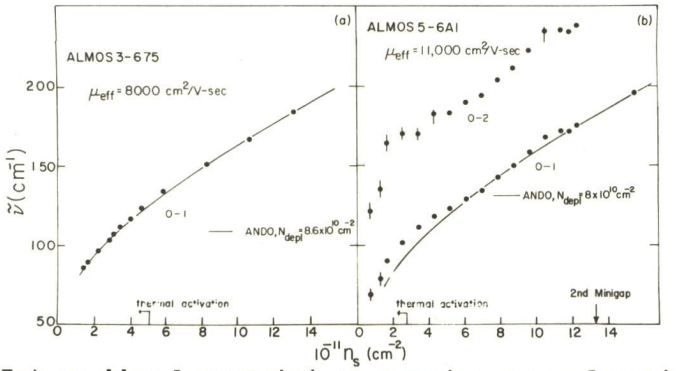

Figure 1 Intersubband transition energies as a function of carrier density for two samples: Solid curves are theoretical results of Ando for two valley occupancy

the two valley state as a function of electron concentration is shown in Fig. (2). The two valley state has higher energy for densities above 2.5×10^{11} cm^{-2} (for the particular depletion charge density, $N_D = 3 \times 10^{11}$ cm^{-2}, used). The value of the crossover density is very sensitive to the exchange-correlation potential. Instead of concentrating on the value of n_c, which we cannot determine with any accuracy, we focus on the fact that the energy difference $\Delta E_{2,6}$ is very small over a large range of density. In addition to the effects of exchange and correlation, we consider the possibility of a spontaneous lattice distortion which lowers the energy of the occupied valleys at the cost of a small increase in elastic energy. The change in energy per particle will be of the form

$$\Delta E_e = \tfrac{1}{2} C e^2 d n^{-1} - \Xi e \quad . \tag{1}$$

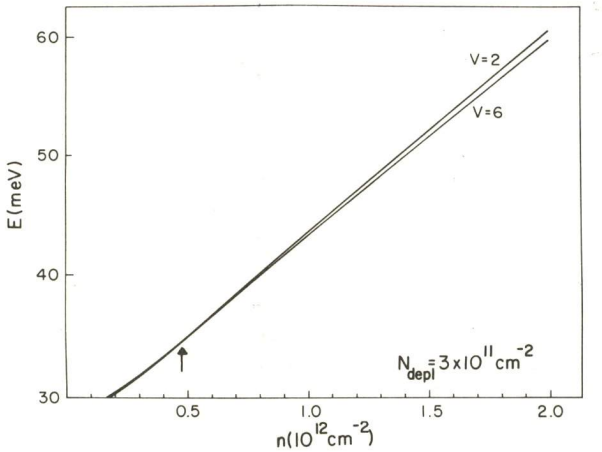

Figure 2 Total ground state energy per particle for six and two valley occupancy vs. density: The arrow indicates the critical density

Here C is an effective elastic constant, e the strain, d the effective thickness of the inversion layer, and Ξ an effective deformation potential. A detailed caluclation of ΔE_e and minimization with respect to strain gives the values shown in Table I.

ΔE_e is not large enough to shift n_c to appreciably higher density, but it does make up a fraction of the energy necessary to stabilize the two valley state at normal "metallic" densities (i.e. $n > 10^{12}$ cm^{-2}).

The remainder of the energy needed to stabilize the two valley state must be due to random uniaxial surface strain as suggested by Tsui and Kaminsky [8]. By including the effects of exchange and correlation and the spontaneous strain, the size of the random surface strain needed to stabilize the two valley state is reduced considerably below the estimate of Tsui and Kaminsky. For example, at $n = 2 \times 10^{12}$ cm^{-2}, we find a random strain of the order of 1.6 meV (a 1 meV shift requires a uniaxial stress of the order of 11 Newtons/mm) as opposed to 6.7 meV if only kinetic energy is considered. For $n = 4 \times 10^{12}$ cm^{-2}, the corresponding strain energies are 4.7 and 13.4 meV respectively.

$n(10^{12}cm^{-2})$	$E_{2,6}$ (meV)	E_e (meV)
0.5	.018	- .031
0.7	.091	- .046
1.0	.227	- .069
3.0	1.47	- .263
5.0	2.96	- .503
7.0	4.57	- .774

Table I $\Delta E_{2,6}$ is the energy separation per particle between two and six valley occupancy. ΔE_e is the energy change per particle due to self-induced strain

Samples with valley degeneracy of six [9] presumably have their stress relieved somehow in the fabrication process and are thus stable against a transition to two valley occupancy at much lower densities. In these samples the E_{10} transition energies are always smaller than those observed on two valley samples at the same electron density [10]. This agrees with our interpretation of the shift in E_{10} caused by a valley occupancy phase transition. We note here that the experiments are done under high magnetic field while our calculation is for zero magnetic field. A strong magnetic field will enhance the transition by quenching the kinetic energy, the principal opposing force to the exchange correlation instability. Recent observation by Englert et al. [11] in the extreme quantum limit, and by Woo and Stiles [12] on Si (111) surfaces which show valley degeneracies other than six are not inherently in disagreement with the current model. At finite temperatures, entropy will favor six valley occupancy and a transition temperature of the order of 10°K is estimated for condensation energy of order 1 meV.

Footnotes and References

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