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Spontaneously Polarized Superlattice: A Novel Quantum Confined Structure with Order/Disorder Phase Transition

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1. Introduction Recent advances in direct observation of electron-wave behavior[1] have stimulated anticipation of unprecedented electron devices, which are beyond the scope of classical device concepts. However, the use of such "novel" devices in actual integrated circuits seemingly will differ only slightly from conventional devices. That is, they must still use classical circuit schemes, in which logic and memory functions are realized with metal-interconnected devices. Based on these visions, quantum effects are expected to be more widely used in information processing hierarchies[2]. An ultimate goal in this direction will be parallel distributed processing by independently controlled electrons[3] (or ordered electrons). However, so far, the motion of electrons in any electron device is random. It is unknown if any kind of electron "order" can be imposed in an actual electron system.

As a first step in pursuit of this goal, this paper proposes and analyzes a semiconductor superlattice structure with spontaneously ordered carriers. Special emphasis is placed on the utilization of impurity-carrier dipoles and their interaction. The dipole interaction has the potential of controlling the motion of each electron even in the mesoscopic scale, due to the relatively long interaction range ($\alpha\ 1/r^3$).

2. Results An example of the proposed spontaneously polarized superlattice (SPS) concept is a 3-D lattice, in which each unit cell contains a pair of quantum boxes (or dots) (Fig. 1). The lattice is embedded in the barrier region. This SPS has the possibility of displaying the following novel electronic states:

(1) All carriers are cooperatively displaced in one direction, without an external electric field (Fig. 4 insert). In other words, a carrier-ordered phase with spontaneous polarization appears. This is because the quantum- box pairs, which easily have dipole moments even with a small electric field, mutually interact with positive feedback.

(2) An order/disorder phase transition occurs at a finite critical temperature. This is because thermally excited carriers favor random distribution.

(3) A strongly correlated motion of many electrons will be observed at around the critical temperature, resulting in a high dielectric constant (ideally the constant diverges).

The probability that these unique properties will appear under the constraints of actual material parameters is numerically analyzed. The basic equations are a self-consistent combination of (1) the Schroedinger equation in the quantum-box pairs, and (2) the dipole interaction formula between different pairs. These equations are solved under various conditions of changes in barrier height and feature sizes.

The eigenstates of quantum-box pairs can be recognized as a two-energy system (pseudo-spin system) having a symmetrical ground state and an antisymmetrical first-excited state (Fig. 2). The two nearly degenerate states at the 0 field separate with an increasing field. This is similar to the spin system in magnetics, in which the Zeeman effect causes energy levels to separate with increasing magnetic field.

The effect of the barrier between quantum boxes is high sensitivity of carrier displacement, even to a very weak electric field. As shown in Fig. 3, sensitivity increases with decreasing temperature, and eventually exceeds the threshold level for spontaneous displacement. The threshold level is determined by the condition in which a kind of "gain" in a feedback loop is unity. The feedback loop consists of an occasionally polarized quantum-box pair, induced dipoles around the pair, the feedback field at the original pair, and the resulting polarization of the pair. Fig. 3 shows that spontaneous polarization occurs under the actual constraints of material parameters of GaAs/AlAs and Si/SiO_2.

Dielectric constant is an index of correlation between carriers. As shown in Fig. 4, dielectric constant increases rapidly with decreasing temperature, and it diverges at a critical temperature (35K in GaAs/AlAs). This means that the correlation of carriers, which are randomly distributed at high temperatures, increases rapidly as the critical temperature is approached, and covers the whole lattice when finally reaching the critical temperature, resulting in a carrier-ordered state. Fig. 4 also shows that similar lattice structures without the barrier between the two boxes show no phase transition even at zero Kelvin. This proves that the high polarizability inherent in the double-minimum potential structure is essential for the formation of the ordered state.

The spontaneous polarization itself is known to occur in ferroelectrics such as KDP [4]. In ferroelectrics, the dipole moment originates from the displacement of ions, which are over 1000 times heavier than carriers in SPSs, and therefore, the response is much slower. The other major difference is that the characteristics of SPSs can be designed by changing the geometry, and other parameters.

In conclusion, SPS is proposed and numerically analyzed to have a carrier-ordered state under actual material parameter constraints. The unique feature of SPS, in which properties are drastically changed by the design of parameters, offers a "phase-transition design" concept, which is a novel and unexplored degrees of freedom in semiconductor material design. SPS is expected to be applied to electron-level parallel distributed processing and opto-information processing.

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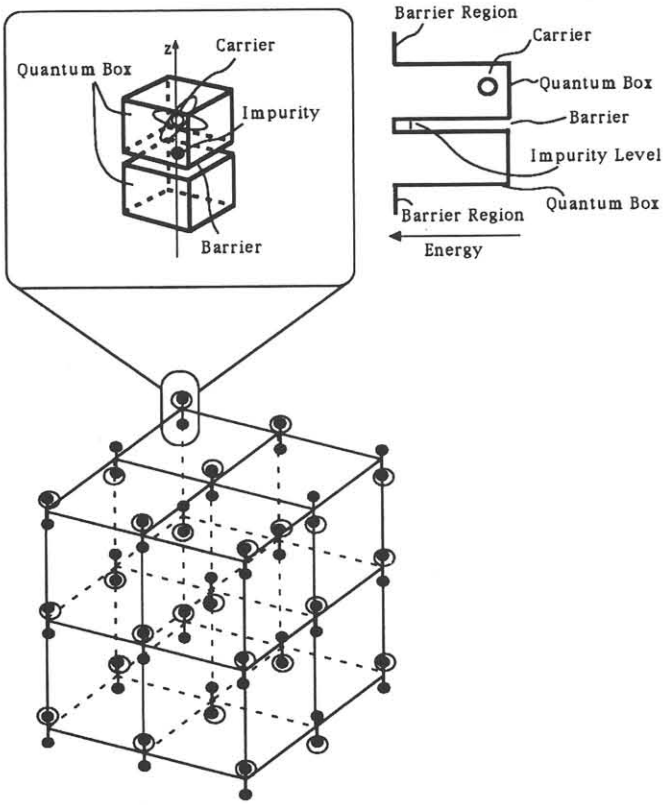

Fig.1 The structure of spontaneously polarized superlattice.

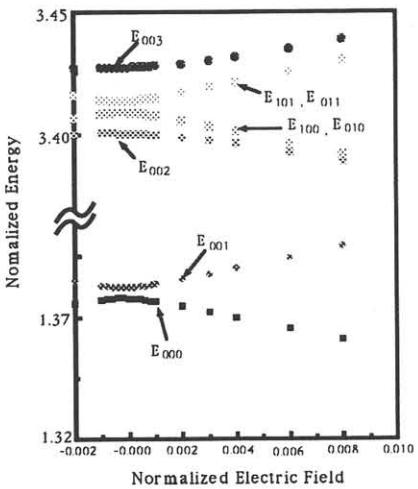

Fig. 2 The dependence of normalized eigenenergy on electric field.

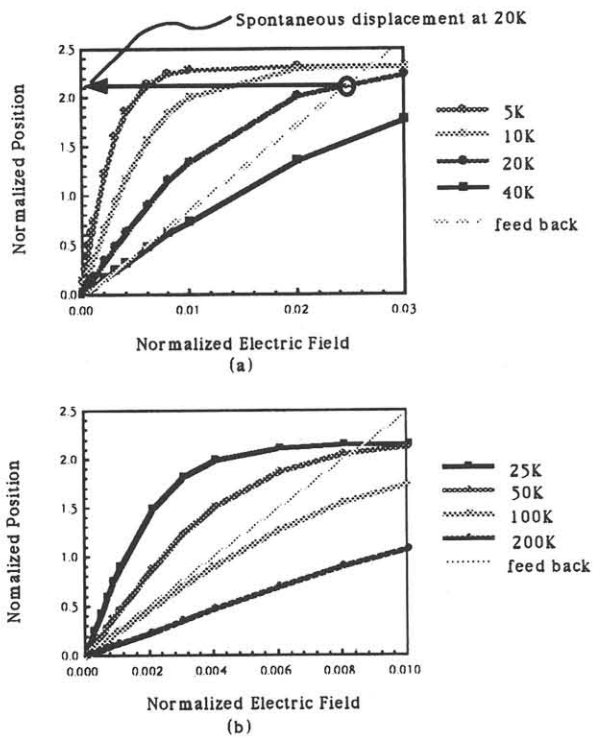

Fig. 3 Normalized displacemant vs. normilized electric field. (a) GaAs/AlAs. Size of quantum box is 3.5nm, thickness of barrier between boxes is 1.67nm, lattice constant is 10nm, unit displacement is 1.11nm, unit electric field is 4.44×10^5 V/cm . (b) Si/SiO2. Size of quantum box is 1.4nm, thickness of barrier between boxes is 0.67nm, lattice constant is 4nm, unit displacement is 0.45nm, unit electric field is 8.61×10^6 V/cm .

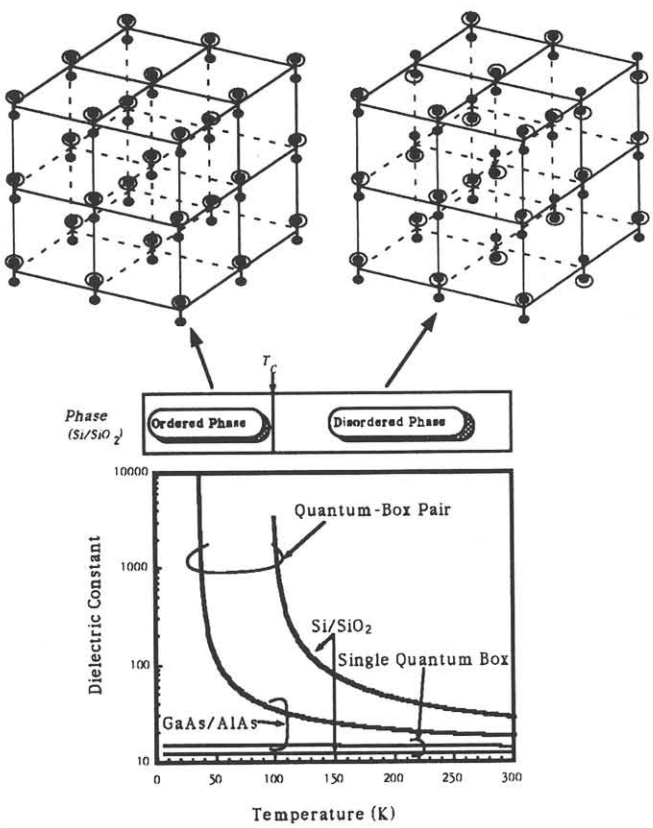

Fig. 4 Temperature dependence of dielectric constant.