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TRANSPORT IN SURFACE SUPERLATTICES ✩

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Transport and scattering in a lateral surface superlattice are investigated. A Monte Carlo calculation of the drift velocity versus electric field, using simple sinusoidal energy bands in two dimensions, shows negative differential mobility. The negative differential mobility is the result of Bloch oscillations, as is apparent from oscillations in the velocity autocorrelation function.

The electronic structure of a semiconductor is intimately connected with the periodicity of the crystal lattice. Various workers have considered the effects of superimposing a second periodicity onto the normal lattice periodicity thus forming a superlattice. Esaki and Tsu [1] developed the current interpretation of one dimensional layered superlattices where, in the most common form, molecular beam epitaxy is used to lay down, e.g., alternate layers of GaAs and GaAlAs. The effect of the superlattice is to open gaps within the conduction band thereby producing a miniband structure. The idea of a superlattice had however been conceptualized earlier. Peierls [2] discussed a general distortional instability that would introduce minigaps in the conduction electron spectrum, and such charge distortion has led to the concept of superlattice-like effects.

In this letter, scattering and transport in a lateral surface superlattice are modeled. While the presence of a lateral surface superlattice at the Si–SiO_2 interface has been suggested by experimental measurements [3], the possibility that surface superlattices may represent the ultimate limitation of very large scale IC's [4] is a main motivation for this work. Here one possible surface superlattice, which could be fabricated by an extension of present laboratory lithographic processes, is studied. The results are expected to apply to a far wider class of structures.

The system investigated here is a three dimensional quantized superlattice formed from cylinders of GaAs being placed in a thin epi-film of GaAlAs in a square lattice array. This thin film epi-layer confines the electrons to the layer. The resulting structure has been discussed extensively elsewhere [5], and differs in several important respects from the commonly studied Esaki superlattice. The Esaki superlattice is a 1-dimensional superlattice in a 3-dimensional system and is fabricated by epitaxial growth of alternating layers of two different materials. The surface superlattice is a 2-dimensional superlattice existing in a quasi-2-dimensional system and would be fabricated by extending the lithographic techniques used to make very dense integrated circuits. While conceptually, and probably technologically, difficult to fabricate, the actual manner of formation of the surface superlattice is not important. The present device can be considered to be a generic surface superlattice, and the effects differ little (discussed below) from those of Bate's MOS array [5,6].

The square lattice array of GaAs cylinders in the

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background of GaAlAs [5] creates a square array of cylindrical potential wells. An LCAO model using only nearest neighbor interactions gives exactly cosinusoidal miniband formation within the conduction band. The thin epi-layer (or high electric field in the direction perpendicular to the surface in MOS arrays [6]) creates widely-spaced discrete energy levels in the third dimension. If the cylindrical potential wells are replaced by a two-dimensional cosinusoidal potential [7], the minibands differ by approximately 5% from the cosinusoidal bands.

The scattering processes for the surface superlattice are calculated for the system of GaAs/GaAlAs. The scattering rates for acoustic and polar optical phonons have been obtained using a two dimensional density-of-states for cosinusoidal energy bands. A Van Hove [8] singularity occurs in the density of states and produces a singularity in the scattering rate. This singularity was removed by including the self-energy corrections due to the phonons [9], which become important in the vicinity of the singularity. The widely-spaced discrete energy levels in the third dimension allows scattering and transport in that direction to be neglected.

In this surface superlattice, as in others, the conduction band splits into subbands. Here the lowest energy subband was nearly flat. Therefore, transport dominantly occurs in the next higher minibands. The energy dispersion in this subband is approximated by:

$$E = E_0 - E_0/2[\cos(k_x D) + \cos(k_y D)] .$$

where $E_0 = 0.05$ eV is the half-width of the energy band and $D \approx 100$ Å is the distance between potential maxima. The satillite valleys and next subband are at energies of 0.2 eV and 0.3 eV, respectively, above the subband considered. Their contribution to the transport of electrons is insignificant since there are no intermediate energies through which the electrons can scatter to aid population of upper bands as in the Esaki model [10].

The overall transport properties of this system are calculated by an ensemble Monte Carlo technique. The results of the simulation are the velocity–field curves and are shown in fig. 1. The lower curve results for a field applied along one of the (10) basis vectors of the square lattice array of cylinders while in the top curve the field is applied along a (11) direction. At low fields, both curves show a linear region as expected for most structures. At approximately 8–10 kV/cm the curves begin to bend over to the peak near 13 kV/cm. As the field is further increased, the velocity begins to decrease and for this model continues to decrease to zero as the field tends to infinity.

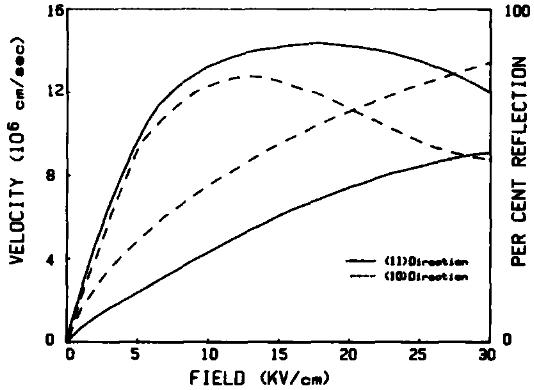

Fig. 1. Drift velocity versus electric field for a lattice temperature of 300 K, and a superlattice spacing of 100 A and miniband width of 100 meV. Full curve, (11) direction; dashed curve, (10) direction. The lower two curves represent the fraction of carriers undergoing Bloch oscillations.

The negative differential mobility is the result of electrons being able to cycle through the reduced Brillouin zone many times before they are scattered. The process of the electrons traveling through an entire reduced Brillouin zone many times before it is scattered has been called Bloch oscillations and can only occur when the energy dispersion is sufficiently narrow to allow a moderate field to move the electrons through the band many times before a scattering event. The percentage of electrons undergoing Bloch oscillations is also shown in fig. 1.

The velocity auto-correlation function is also obtained from the Monte Carlo calculation. The correlation function clearly shows the existence of Bloch oscillations as can be seen in fig. 2. In the low to moderate field region, the velocity correlation function shows the usual shape of a correlation function for parabolic bands. At high fields, however, subsidiary peaks appear at multiples of the time period necessary for an electron to cycle through the entire energy band. Also, as expected, the period of the oscillations decrease as the accelerating field is increased.

The upper frequency bound of this ndm is expected to exceed that of either Gunn devices or

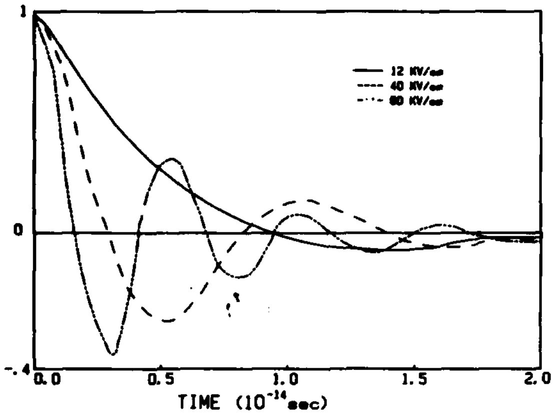

Fig. 2. The velocity autocorrelation function for electrons in the surface superlattice. At the higher field, oscillations in the correlation function occur at times corresponding to multiples of the Bloch oscillator period.

real-space transfer devices. First, the ndm obtained here does not arise from intervalley Gunn effects or from a diffusive "real space" transfer between material layers. Furthermore, the energy and momentum relaxation processes occur much more rapidly in the surface superlattice than in the bulk material. Therefore, surface superlattices may become useful sources at high millimeter and submillimeter wavelengths, especially due to their planar nature.

In summary, transport and scattering in a generic surface superlattice structure have been investigated. A negative differential mobility arising from Bloch oscillations was found. The surface superlattice negative differential mobility is expected to be useful at much higher frequencies than that due to the conventional Gunn effect. Alternatively, related instabilities may be an ultimate limit on very large scale integration [7,10].

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