Influence of a natural superlattice from a surface with high indices on the spectrum of $2D$ electrons in a multivalley semiconductor

V. A. Volkov and V. B. Sandomirskiĭ

Institute of Radio and Electronics

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We consider the influence of a silicon surface with high indices on the spectrum of a two-dimensional ($2D$) electron gas in an inversion surface layer. Simultaneous allowance for the superperiod in the natural surface lattice and the multivalley character makes it possible to account quantitatively for the experimental data and predict new effects.

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The last decade has seen rapid progress in the investigation of the properties of a $2D$ electron gas in inversion layers produced on semiconductor surfaces in the case of strong bending of the bands.[1,2]

A method of producing a surface superlattice (SL) by cleavage of a crystal along a plane with high Miller indices was proposed in[3]. Such a SL should lead to the appearance of minigaps in the spectrum of the $2D$ electron gas near the surface. This idea was realized simultaneously and independently[4] in an n-type inversion layer on (118) Si.

By now, the Si surfaces (118),[4] (115),[5] (2,2,23),[5] (119)[6] have already been investigated. The observed singularities were attributed to the existence of a gap that appears in the $2D$ electron spectrum when the Fermi level E_F passes through it. The

TABLE I.

Si surface	A, Å	L_{exp} Å	L_{theor}, Å
(1 1 5)	10	~70	66
(1 1 8)	31	101 – 107	104
(1 1 9)	18	110 – 120	116
(2 2 23)	89	~ 200	223

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appearance of the gap was attributed in[4,5] to the presence of a surface SL. However, the crystallographic period A of the SL and the experimental $L=\pi/k_F$ (k_F is the Fermi momentum at which E_F crosses the midpoint of the gap) differ greatly (second and third columns of Table I).

As a result, a different mechanism of gap formation, not connected with the SL, was proposed in[6]. A critical discussion of the theory of[6] is given below.

The purpose of the present paper is to present a brief exposition of the results of a consistent theory of SL in a multivalley semiconductor. An SL with period A, which for the sake of argument is one of the lattice vectors, should give rise to minigaps whose positions are determined in the weak-coupling approximation by the condition $k_m=\pi m/A$ (m is an integer), with the quasiwave vector k_m measured from the center of the Brillouin zone rather than from the center of the valley, as is done in the usual variant of the effective-mass method.[4,5] The observed period π/k_F (k_F is measured from the center of the valley) should not coincide in any way with the true one.

Consider a crystal bounded by an atomic plane. It has a $2D$ symmetry determined by the symmetry of the surface lattice. This influences strongly the spectrum of the states localized near the surface. For $(11n)$Si, the Bravais $2D$ lattice is a primitive rectangular one for even n and a centered rectangular one for odd n. Therefore the Brillouin $2D$ zones for these two cases differ noticeably in size. The ground state in the inversion layer on $(11n)$Si stems at $n \gg 1$ from two ellipsoids centered at the point $\pm K_0$ [001] in the $3D$ Brillouin zone. The corresponding equal-energy ellipses are not shown in Fig. 1, for the sake of clarity, for the first $2D$ Brillouin zone, $\theta=\arcsin\sqrt{2/(2+n^2)}$ is the angle between (001) and $(11n)$. The centers of the ellipse fall in the second (even n) or first (odd n) $2D$ Brillouin zone. Discontinuities appear in the electron spectrum when the Fermi ellipse is tangent to the boundaries of the m-th $2D$ Brillouin zone. The corresponding values of k_F for the even and odd n are determined by the formulas

$$k_F^{(m)}(\text{even}) = \left|\frac{\pi m \sin\theta}{a} - K_0 \sin\theta\right|, \quad k_F^{(m)}(\text{odd}) = \left|\frac{2\pi m \sin\theta}{a} - K_0 \sin\theta\right|, \tag{1}$$

a is the fcc lattice constant ($a=5.43$ Å for Si).

The comparison with experiment is best carried out for the pseudoperiod $L^{(m)}=\pi/k_F^{(m)}$. In Si ($K_0=0.85\times 2\pi/a$) the gaps with the lowest energies correspond to $L^{(2)}$(even) and $L^{(1)}$(odd), in good agreement with experiment (see Table I).

We can consider analogously the surface (2, 2, 23)Si, for which the $2D$ Brillouin zone is a rectangle with the long edge $2\pi\sqrt{2}/a$ along $[\bar{1}10]$ and the short edge $\pi \sin\theta/a$ along $[2\bar{3}\ 2\bar{3}\ 4]$, with $\theta=7°$. The centers of the ellipses fall in the third $2D$ Brillouin zone. The discontinuities in the spectrum correspond to the pseudoperiods $L^{(m)}=2a/(\sin\theta\,|m-3.4|)$.

We succeeded so far in recording in the experiment one gap each for the surfaces indicated in Table I. Let us estimate the concentrations $N^{(m)}$ needed for E_F to reach the next gaps in energy. For (118)Si the next gap with $L^{(1)}$(even)$=45$ Å can be reached

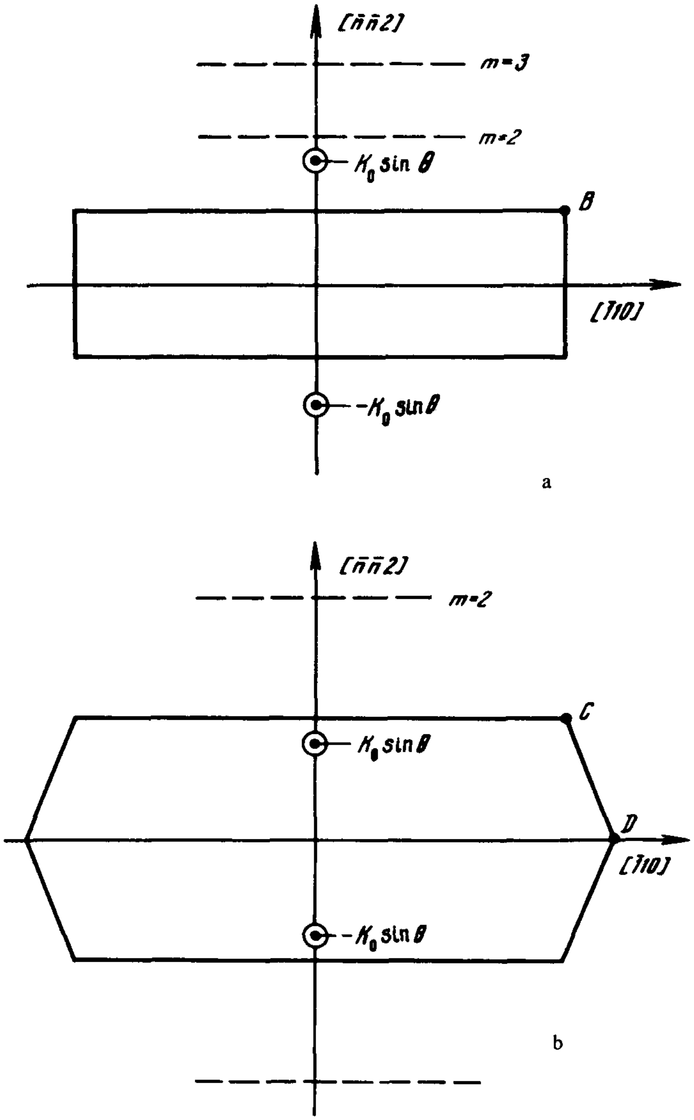

FIG. 1. First $2D$ Brillouin zones for $(11n)$Si: a) even n, b) odd n. The dashed lines mark the boundaries of the next Brillouin zones. $B=(\pi/a)(\sqrt{2},\sin\theta)$; $C=(\pi/a)(\sqrt{2},2\sin\theta)$; $D=[\pi\sqrt{2}(n^2+3)/a(n^2+2),0]$.

at $N^{(1)}(\text{even})=1.6\times10^{13}\ \text{cm}^{-2}$, which is perfectly realistic. For (2, 2, 23)Si, the lowest gap is with $m=3(L^{(3)}=223\ \text{Å}$, $N^{(3)}=6\times10^{11}\ \text{cm}^{-2})$, and with increasing N one should reach gaps with $m=4(L^{(4)}=149\ \text{Å}$, $N^{(4)}=1.4\times10^{12}\ \text{cm}^{-2})$ and $m=2(L^{(2)}=74\ \text{Å}$, $N^{(2)}=6\times10^{12}\ \text{cm}^{-2})$. We note also that it follows from (1) that K_0 can be determined from measurements of $L^{(m)}$.

The foregoing estimates explain clearly why SL effects were not observed in inversion layers of p-type on (115) and (118) of Si.[4] Inasmuch as the extremum of the valence band is located at the center of the Brillouin zone ($K_0=0$), there should have been observed a true period A corresponding to too large a value of N. However, $A=89$ Å even for (2, 2, 23)Si, and the SL effects should be observed at realistic N.

There is also another explanation of the appearance of a gap in the spectrum. It was noted in[6] that the electron dispersion in an n-type inversion layer on $(11n)$Si can be represented at $n \gg 1$ in the form of two closely located parabolas. The intervalley interaction splits the parabolas at the point of their intersection and produces a gap with a pseudoperiod $L=a/0.3\sin\theta$. Formally, the position of this gap coincides with the lower gaps obtained from (1) for $(11n)$Si. The good agreement of the model of[6] with experiment for $n=5$, 8, and 9 is in our opinion accidental. For example, were $K_0<0.75\times 2\pi/a$ satisfied, there would be no longer agreement for even n (the lower gap would be with $L^{(1)}$(even) which is not described by[6]. In addition, for (2, 2, 23)Si the theory of[6] yields $L=149$ Å. This value is in worse agreement with experiment than our values (see Table I) and corresponds in our notation to the higher-energy gap with $L^{(4)}$. Inasmuch as the real 2D symmetry of the Si surface was not taken into account in[6], this model does not lead at all to discontinuities in the spectrum for inversion layers of p-type. We therefore regard the theory of[6] as inconsistent. Of course, the final word belongs to experiment.

The developed approach is applicable also to other similar situations: artificial SL in multivalley semiconductors, magnetic surface levels, surface phonons, plasmons, etc.

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