Electron transmission through silicon stacking faults

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We use a recently developed formalism [Phys. Rev. B **38**, 2021 (1988)] to calculate electron transmission through silicon stacking faults. These systems are of interest both because of their effect on transport in silicon and because they can be viewed as prototypical heterostructures consisting of two different orientations of silicon.

Silicon stacking faults are commonly found near silicon–silicon-dioxide interfaces often bridging two partial dislocations.[1] By scattering electrons, these defects degrade electronic properties near the interfaces. Most theoretical studies of stacking faults have focused on the energetics of their formation;[2,3] in this study we consider their effect on transport. Electron scattering by stacking faults in copper, which was considered by Bross,[4] was found to be quite weak. An important difference between copper stacking faults and those in silicon is that the electrons of interest in copper are those near the Fermi level and in silicon they are those near the conduction-band minimum. Defects like stacking faults tend to scatter electrons much more strongly near band extrema. We also consider generalized stacking faults, which we will define below, because they illustrate in a simple system some of the properties of more complicated heterostructures.

Intrinsic stacking faults, shown in Fig. 1, result from the removal of the facing halves of two adjacent double layers and subsequent rebonding; extrinsic stacking faults, also shown in Fig. 1, result from the insertion and rebonding of two additional halves of double layers. Alternatively, these two structures can be constructed by separating two twist boundaries by one or two double layers, respectively. Pseudopotential calculations by Chou *et al.*[2] show that the forces on the atoms in these ideal structures are small and will not lead to significant atomic rearrangements.

Evanescent states play two important roles in electron transmission through these interfaces. The first is to provide the necessary degrees of freedom to satisfy the wave-function matching conditions when calculating the transmission across the simple constituent interfaces, the twist boundaries.[5] In addition to giving a discontinuous wave function, a matching process which excludes the evanescent states gives transmission probabilities that differ greatly from the correct result. The second role results from their finite decay length. For a compound interface like a stacking fault (consisting of two twist boundaries), the evanescent states associated with each simple interface will effect the transmission through the other. To better understand this second effect, we will consider both the stacking-fault structures discussed above and generalized stacking faults which are constructed in the same way, but with an arbitrary number of double layers separating the two twist boundaries.

We calculate transmission probabilities for these structures in two ways, a full calculation similar to that done for the twist boundary[5] and an approximate calculation based on the results of isolated twist-boundary calculations. Comparing the two results shows the effect evanescent states associated with one interface can have on transmission though a neighboring interface.

Briefly, the full calculation proceeds in the following manner. The structure is divided into layers, and we compute the potential in each layer using a linear augmented-plane-wave (LAPW)–based local-density-functional calculation.[6] Using this potential and LAPW basis functions, we find a set of linear relations[7] between the bounding-plane values and slopes of variational solu-

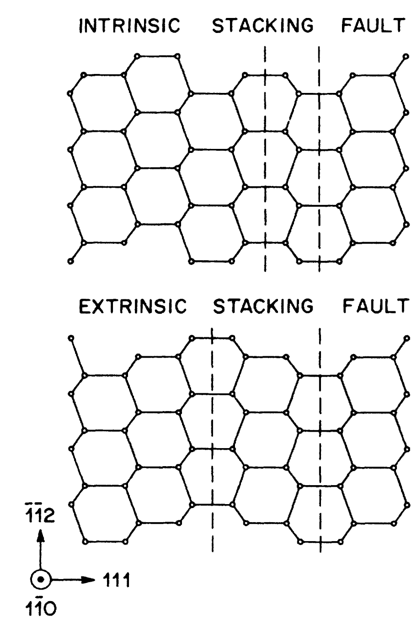

FIG. 1. The structure of stacking faults in silicon, shown projected along the $[1\bar{1}0]$ direction. The long lines represent bonds lying in $(1\bar{1}0)$ planes, while short lines are bonds connecting atoms in neighboring $(1\bar{1}0)$ planes. The dashed lines are twist boundaries which can be viewed as making up the stacking faults.

tions of the Schrödinger equation for that layer. For the bulklike layers, these relations lead to a set of generalized Bloch states which allow us to join an infinite number of layers together with scattering-state boundary conditions at infinity. These generalized Bloch states are matched together through the joining regions, here the reversed-orientation silicon, to construct the electron scattering states for the entire structure of interest.

We compare the full calculation of the electron transmission with an approximate calculation that is based on previous results for isolated twist boundaries[5] and that ignores the affects of the evanescent states from one such interface on the other. The full twist-boundary calculation gives a state

$$\psi(\mathbf{r})=\left[\psi_{\rm in}(\mathbf{r})+R\,\psi_{\rm refl}(\mathbf{r})+\sum_i \psi^i_{\rm decay}(\mathbf{r})\right]\theta(-\mathbf{r}) + \left[T\psi_{\rm trans}(\mathbf{r})+\sum_i \psi^i_{\rm decay}(\mathbf{r})\right]\theta(z) \tag{1}$$

that consists of an incident Bloch state $\psi_{\rm in}$, a reflected Bloch state $\psi_{\rm refl}$, a transmitted Bloch state $\psi_{\rm trans}$, and evanescent contributions that decay away from the interface in either direction $\psi^i_{\rm decay}$. For the approximate calculation, we use the transmission amplitude T and the reflection amplitude R calculated using all of the evanescent states for matching at each isolated interface, but then ignore the evanescent contributions to the wave function in the process of joining the two.

For an isolated twist boundary it is necessary to include the evanescent states in the matching to get the transmission probability correct for all energies except the band minimum. Right at the band minimum, the incident and reflected states are matched perfectly to each other and the transmitted state is poorly matched to either so that the matching conditions can be satisfied with just the first two states, giving no transmission.[5] As the incident energy increases [see Fig. 2(f)], the transmission probability increases until it becomes unity about 0.13 eV above the conduction-band minimum. If the evanescent states are not included in the matching, the transmission probability remains close to zero over that entire range.

Using the twist-boundary results we consider the multiple reflection, transmission, and Bloch propagation of an electron in a structure with two twist boundaries separated by n double layers of thickness a. The transmission amplitude is found by summing the transmission amplitudes for each of the multiple reflections and transmissions

$$T_n=T_1T_2e^{ik_{z1}na}(1-R_2\tilde{R}_1e^{i(k_{z2}+k_{z1})na})^{-1}\,, \tag{2}$$

where k_{z1} and k_{z2} are the wave vectors for the right- and left-moving Bloch states in the layers between the twist boundaries. The transmission amplitudes for electrons incident from the left are T_1 and T_2 for the first and second interfaces, respectively. The reflection amplitudes for right- and left-moving electrons inside the reversed silicon are $\tilde{R}_1$ and R_2. All of these quantities are energy dependent.

Figure 2 compares this approximate calculation with the full calculation for structures with different numbers of double layers separating the twist boundaries. Figure 2(a) shows the transmission probability for the intrinsic stacking fault; for low energies, transmission is much more likely than it is for an isolated twist boundary. In addition, there is a large difference between the full and the approximate calculation. These results imply that interaction of the evanescent states associated with each interface tends to "bridge" the reversed region, carrying the incident wave through to the (identical) transmitted wave with less distortion. The state has not completely adapted to the reversed crystal structure before it encounters the second interface. The results for the extrinsic stacking fault, shown in Fig. 2(b) are qualitatively similar to the results for the intrinsic stacking fault except that the transmission probability is closer to that for the twist boundary and the discrepancy between the full and the approximate calculation is reduced. Both of these differences result from the greater decay of the evanescent states between the more widely separated twist boundaries. The decay constants of the most slowly decaying evanescents are given in Fig. 3.

In Fig. 2(c), which shows the transmission probability for a structure with four double layers between the two twist boundaries, the difference between the two calculations has become much smaller. At this separation the amplitude of the most slowly decaying evanescent state

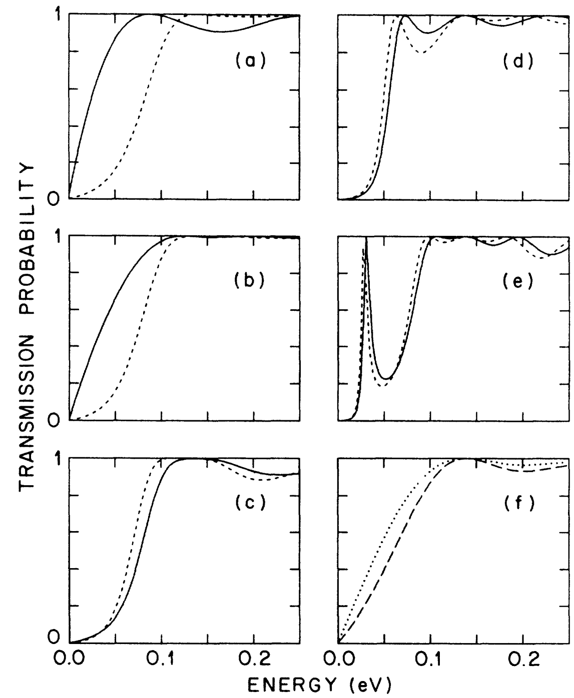

FIG. 2. The transmission of electrons through silicon stacking faults. (a)–(e) show the transmission probability through stacking faults consisting of two twist boundaries separated by 1, 2, 4, 8, and 16 double layers of reversed-orientation silicon. The solid curves are the results of a full calculation, and the dashed curves are the results of the approximate calculation described in the text. (f) shows the transmission through a single twist boundary (dotted curve) and the incoherent transmission (long-dashed curve) through two twist boundaries.

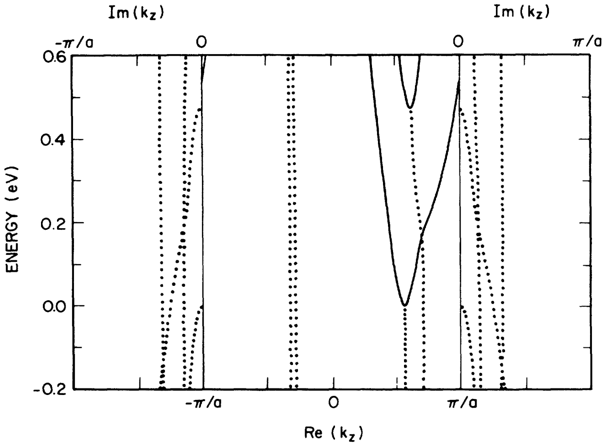

FIG. 3. A detail of the [111]-direction silicon complex band structure near the conduction-band minimum. The center panel shows the real, and the left- and right-hand side panels the imaginary parts of the wave vectors of the most important generalized Bloch states for energies near those used in Fig. 2. The wave vector parallel to the interface is that of the conduction-band minimum projected onto a (111) plane. The layer spacing a is $a_{\text{cubic}}/\sqrt{3}$. The solid lines (in the center panel) give the wave vectors of the propagating states, and the dotted curves give the real and imaginary parts of the evanescent states.

from the first interface has decayed by a factor of 0.16 at the second interface. For silicon structures in which substructures are separated by more than four double layers, we would expect that the effect of evanescent states from one substructure on the others could be ignored in calculating the electronic properties. However, this will not be the case if long-range rearrangements of the lattice occur or if there are long-range changes in the electronic potential, both of which can change the appropriate decay constants.

The agreement between the two calculations continues to improve as the number of reversed double layers increases to eight and 16 as shown in Figs. 2(d) and 2(e). These panels also show the existence of "Fabry-Perot" transmission resonances; these occur when the electronic phase changes by 2π on one full circuit of the region between the two twist boundaries. Note that to correctly predict the resonance positions, it is necessary to include the phase change involved in the reflections; ignoring that phase change would predict resonances at 0.06, 0.17, 0.24, and 0.34 eV for the 16 double-layer structure rather than the observed resonances at 0.03, 0.11, 0.19, and 0.28 eV. The apparent resonance at 0.14 eV is due to the unit transmission probability for the isolated twist boundary. As is expected, the resonances are narrower where the twist-boundary reflection is stronger, at lower energies.

The agreement between the full and approximate calculations for the 16 double-layer structure becomes worse as the energy increases because the decay length of the slowest decaying evanescent state increases with increasing energy, as can be seen in Fig. 3. The unit transmission at 0.14 eV is associated with a change in character of the generalized Bloch states that is reflected in the change in slope of the conduction band and of one of the evanescent states seen in Fig. 3. At this energy the band states and the evanescent states mix with each other as can be seen by comparing probability and flux distributions for the states.

As the twist boundaries get further and further apart, the resonances will become closer and closer together. At some point the energy resolution of the incoming electron state will be smaller than the inverse energy separation of the resonances, and the resonances will be effectively averaged over. In this situation, the twist boundaries will scatter incoherently which leads to the transmission probability shown in Fig. 2(f). This transmission probability is always less than the transmission probability for the isolated twist boundary.

In summary, we have calculated transmission probabilities for a series of generalized silicon stacking faults. Intrinsic and extrinsic stacking faults scatter electrons much more weakly than an isolated twist boundary. This decreased scattering is due to the evanescent states associated with the matching at each twist boundary affecting the transmission through the other. For more widely separated interfaces this effect becomes much smaller, as would be expected from the decay constants of the evanescent states. In addition, these more widely separated structures show sharp transmission resonances when there is constructive interference for the multiple reflections between the twist boundaries.

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[1]L. F. Ray and D. J. H. Cockayne, Philos. Mag. **22**, 853 (1970).

[2]M. Y. Chou, S. G. Louie, and M. L. Cohen, Phys. Rev. B **32**, 7979 (1985); in *Proceedings of the Seventeenth International Conference on the Physics of Semiconductors, San Francisco, 1984,* edited by J. D. Chadi and W. A. Harrison (Springer-Verlag, New York, 1985), p. 43.

[3]L. F. Mattheiss and J. R. Patel, Phys. Rev. B **23**, 5384 (1981); J. Sanchez-Dehesa, J. A. Verges, and C. Tejedor, *ibid.* **24**, 1006 (1981); S. Marklund, Phys. Status Solidi **108**, 97 (1981); Z. Zhao-bo and L. Jin-ling, J. Phys. C **19**, 6739 (1986); G. Xingao and Z. Qing-qi, Solid State Commun. **62**, 65 (1987).

[4]H. Bross, J. Phys. F **12**, 2883 (1982).

[5]M. D. Stiles and D. R. Hamann, Phys. Rev. B **38**, 2021 (1988).

[6]L. F. Mattheiss and D. R. Hamann, Phys. Rev. B **33**, 823 (1986).

[7]G. Wachutka, Phys. Rev. B **34**, 8512 (1986).