Structure, barriers and relaxation mechanisms of kinks in the 90° partial dislocation in silicon

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Kink defects in the 90° partial dislocation in silicon are studied using a linear-scaling density-matrix technique. The asymmetric core reconstruction plays a crucial role, generating at least four distinct kink species as well as soliton defects. The energies and migration barriers of these entities are calculated and compared with experiment. As a result of certain low-energy kinks, a peculia alternation of the core reconstruction is predicted. We find the solitons to be remarkabl even at very low temperature, and propose that they mediate the kink relaxation dyn

61.72.Lk, 71.15.Pd, 71.15.Fv

The importance of dislocations in semiconductors hardly needs comment. In addition to being responsible for plastic behavior in general, dislocations occur com mnly at semiconductor interfaces where they can act ttering centers for carriers. In sil- ts of 60°-edge

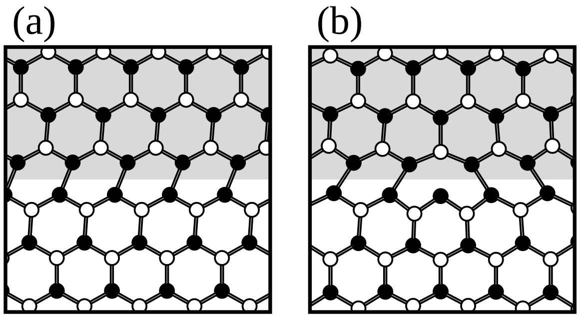

FIG. 1. (a) Top view of the slip plane of a reconstructed 90° partial dislocation. The shaded area indicates the stacking fault. Horizontal and vertical directions correspond to $[1\bar{1}0]$ and $[11\bar{2}]$ directions, respectively. (b) Reconstruction defect, or soliton, where the core reconstruction changes orientation.

nal line minimization performed exactly [11]. Ground-state structures were computed by allowing all atomic coordinates to relax fully (forces less than 5 meV/Å). ed will be described below, all energies are given with

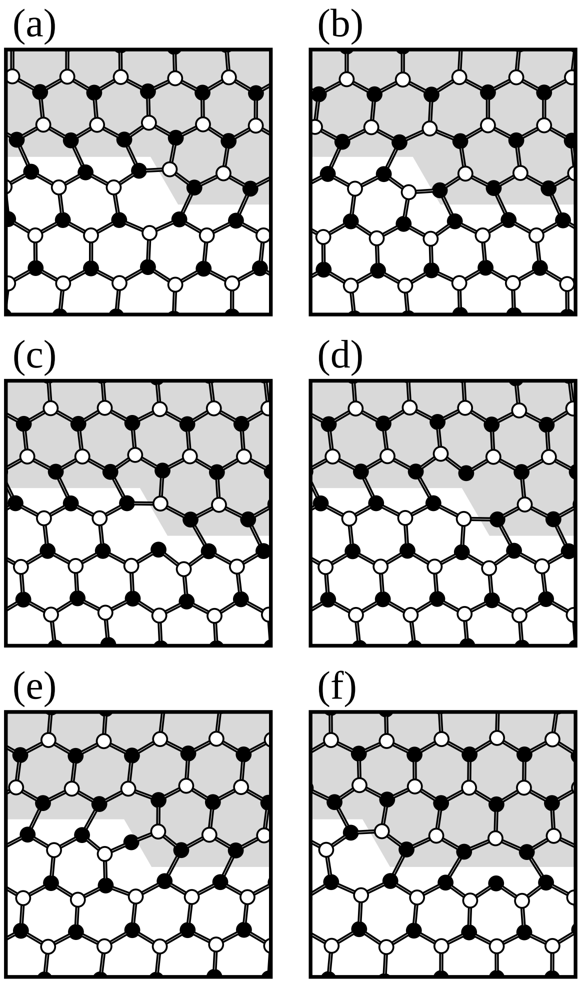

FIG. 3. Core structure of various kinks and a kink-soliton complex. Kink notation relates to bond reconstruction on each side of the defect, and is explained in the text. (a) RL kink. (b) LR kink. (c) LL kink. (d) LL* kink. (e) RR kink. (f) LR kink + soliton.

right-left (RL) kink, the notation following accordingly

for the other types. The above supercell was used to

the energies for the LR and RL kinks. The lat-

"kink vector" [14],

TABLE I. Calculated formation energy for defects in the core of the 90° partial dislocation in silicon. Included also are the migration barriers for a soliton and the low energy kinks.

	Formation energy (eV)	Migration barrier (eV)
soliton	1.31	0.04
LR kink	0.50	1.87
RL kink	0.50	1.83
LL kink[a]	1.74	—
LL* kink[a]	1.76	—
RR kink	2.04	—
soliton + LR kink	1.68	—
soliton + RL kink	1.63	—

[a] Approximate energy. Defect is unstable

of the size of the kink formation energies and migration barriers, and make a connection with the experimental s. For the velocity of a gliding dislocation we have,

$$W_m)/kT] \, , \qquad (5)$$

k and W_m is