"electronic additions" (i.e. surface adatoms or vacancies) that lead to electronic compensation and thus to

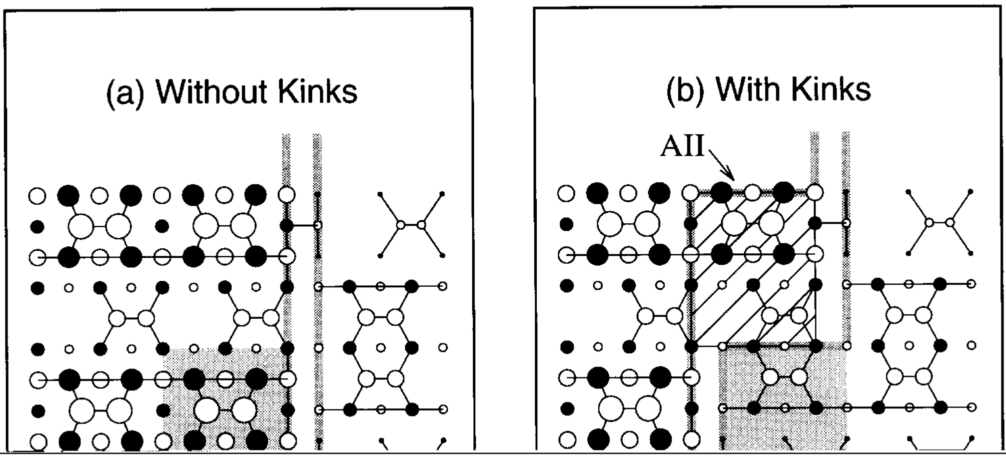
stable and semiconducting flat surfaces. While step–step interaction has noticeable effects on step formation energies, the formation of steps is generally endothermic. There are two commonly observed steps: those with edges parallel to the direction of surface As

Previous studies of GaAs(001) surfaces [17] revealed that the octet rule tends to be obeyed by these

motifs, leading to a set of point charges on various surface atoms. For example, Ga has 3 valence electrons, so fourfold coordinated $Ga^{(4)}$ contributes 3/4 electrons to each of its four bonds. This leads to local charge neutrality. Planar $Ga^{(3)}$ is a 3/4 electron donor

Table 1
Coefficients $\omega_M(\sigma)$ denoting the frequency of motif M, coefficients N_R of the chemical potential terms in structure σ for (i) point defects, (ii) (001) surfaces and (iii) $(001)-2\times4$ surface steps of GaAs and appropriate energies

	$\omega_M(\sigma)$ for the following								N_R for the following					
(i) Defects (per defect)														
(1) $V_{Ga}{}^{3-}$	−1	−4	0	4	0	0	0	—	3	1	0	0.52	Fitted	5.78
(2) $V_{As}{}^{3+}$	−4	−1	4	0	0	0	0	—	3	−1	−1	0.52	Fitted	0.77
(3) $Ga_{As}{}^{2-}$	1	−1	0	0	0	0	0	—	−2	−2	−1	0	Fitted	2.45
(4) $As_{Ga}{}^{2+}$	−1	1	0	0	0	0	4	—	2	2	1	0	Fitted	1.98
(ii) Surfaces (per 1 × 1)														


(a) Without Kinks
(b) With Kinks
AII

4.2. Stability of A steps vs. B steps

As mentioned in Section 3.4, Heller et al. [5] have measured step energy by way of measuring the kink distribution on GaAs(001)-2×4. Depending on temperature, they obtained an A step formation energy

include also the corner energies in Ref. [5]). Following Heller et al., one may derive from the calculated kink energy in Section 3.4 the A step formation energy. This gives 28–31 meV/(1×). Heller et al. also determined the B:A energy ratio to be 5.6–6. Ide et al. [7], on the contrary, estimated the ratio from measured aniso-

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References

[1] P.M. Petroff, A.C. Gossard and W. Wiegman, *Appl. Phys. Lett., 45* (1984) 620.
[2] A. Gomyo, T. Suzuki, S. Iijima, H. Hotta, H. Fujii, S.