Surface Science: Foundations of Catalysis and Nanoscience
List of corrections to first printing

Chapter 1

Fig. 1.1. The second layer in the fcc(110) lattice is misplaced. It should look like the following:

$[\bar{1}10]$

Second layer

First layer

$[00\bar{1}]$
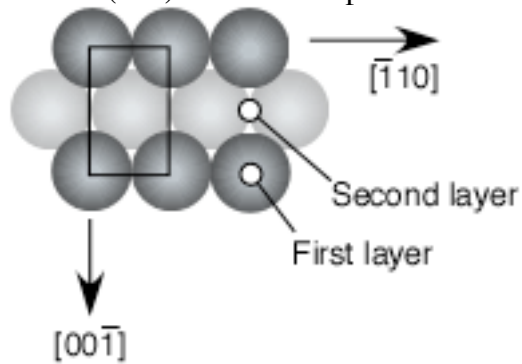
(c) fcc(110)

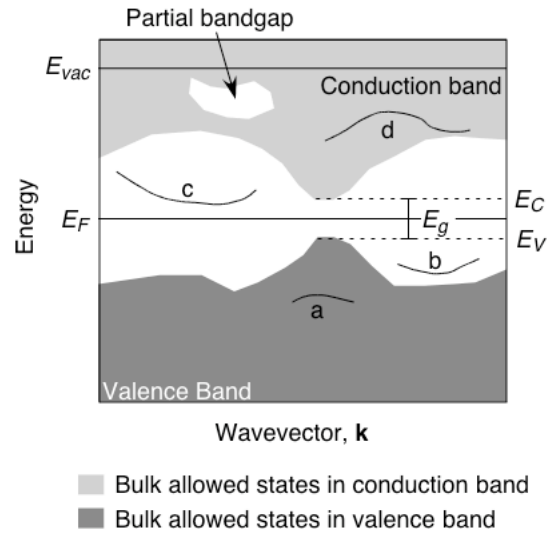Fig. 1.3 (a) hcp(0001) = (001).

Fig. 1.15 Can't see state a.

Fig. 1.15

p. 19 Should read:
In Fig. 1.13(a) the metal has donated charge to the semiconductor space-charge region. The enhanced charge density in the space-charge region corresponds to an **accumulation layer**. In Fig. 1.13(b) charge transfer has occurred in the opposite direction. Because the electron density in this region is lower than in the bulk, this type of space-charge region is know as a **depletion layer**.

p. 26
1.2. Redraw Fig. 1.13 for a *p*-type semiconductor.[17, 19]

Note correction to references.

p. 27

$$\langle u^2 \rangle = \frac{3N_A \hbar^2 T}{M k_B \theta_D^2} \tag{1.31}$$

Note typo in Eq (1.31). The variable should be N_A (Avagadro constant) not N and m should be M, the molar mass.

1.6. The surface Debye temperature of Pt(100) is 110 K. Take the definition of melting to be when the fractional displacement relative to the lattice constant is equal to ~8.3% (**Lindemann criterion** [28,29]). What is the surface melting temperature of Pt(100)? What is the implication of a surface that melts at a lower temperature than the bulk?

NB: The Lindemann criterion is 8.3% not 25% as found in the book. Note new references.

[28]   JJ Gilvarry, Phys. Rev. **102** (1956) 308.
[29]   FA Lindemann, Phys. Z. **11** (1910) 609.

Chapter 2

p. 48

$$m_{12} = \frac{-1}{\det \mathbf{M}*} m_{21}^*$$

(2.21)

$$m_{21} = \frac{-1}{\det \mathbf{M}*} m_{12}^*$$

(2.22)

p. 51. The caption to Fig. 2.16 is uniquely inconsistent with the figure. It should read:
    Fig. 2.16 Some commonly observed adsorbate structures on low-index face-centred cubic(fcc) planes. (a) fcc(111), (i) (1×1), (ii) (2×2), (iii) (√3×√3). (b) (i) fcc(100)–c(2×2), (ii) fcc(110)–c(2×2). (c) (i) fcc(100)–(2×2), (ii) fcc(110)–(2×1).

p. 74

$$T = 10^{-acl} = \exp(-\alpha l)$$

(2.66)

$$\alpha = 2.3026 \ ac$$

(2.67)

Chapter 3

$$\delta E = \frac{4\mu}{(1+\mu)^2}(E_i + q_{ads})$$

(3.26)

Eq. (3.26) has been corrected to put the square in the proper place.

$$N_{vJ} = N_v \frac{hc}{k_B T}(2J+1)\exp\left(\frac{-E_{rot}}{k_B T}\right),$$

(3.30)

In Exercise 3.8, typo referred to Exercise 3.1 instead of 3.7. Eq. (3.36) should read

$$\langle E_{vib} \rangle = \sum_{n>0} \frac{h\nu_n}{\exp(h\nu_n / k_B T) - 1}.$$

(3.36)

Note that this neglects the contribution of zero-point energy to the vibrational energy.

In Exercise 3.14, typo in book reads S_d instead of s_o and a minus sign is missing in the exponential term.

$$s_0 = A_s \exp(-E_a / RT),\qquad(3.37)$$

There is a typo in Table 3.7 in the book. Most of the values for Cu and Si have been switched.
Table 3.7

T_s (K)	$\langle E_{rot}\rangle$ (K)	T_{vib} (K)	$\langle E_{trans}\rangle$ (K)	E_{ads} (eV)
D_2/Cu(111): 925	1020	1820	3360	0.5
D_2/Si(100): 780	330	1700	960	0.8

$$M_i = \int_0^\infty v^i f(v)\,dv.\qquad(3.41)$$

Eq. (3.41) has been corrected such that v is raised to the ith power.

Chapter 4
pp. 179–180. The discussion should simply be improved. This correction messes with the subsequent equation numbers.

To define more precisely what we mean by the activation energy and how it relates to the PES, we turn to Fig. 4.5. First we note, as shown by Fowler and Guggenheim [1], that the activation energy, in this case E_{des}, is given by the difference between the mean energy of the reactants $\langle E\rangle_R$ and the mean energy of the molecules in the transition state $\langle E\rangle_{\ddagger}$

[1] R. H. Fowler and E. A. Guggenheim, *Statistical Thermodynamics*. Cambridge University Press, Cambridge, UK, 1939.

$$E_{des} = \langle E\rangle_R - \langle E\rangle_{\ddagger}\qquad(4.52)$$

Since both $\langle E\rangle_R$ and $\langle E\rangle_{\ddagger}$ are temperature dependent, E_{des} is, in principle, also temperature dependent. The classical barrier height on the PES is $E_{0,des}^c$. E_{des} is not simply related to $E_{0,des}^c$. As can be seen in Fig. 4.5, the two energies are identical at 0 K. At any other temperature, E_{des} and $E_{0,des}^c$ are different, though they likely have similar values.

To account for this expected temperature dependence, it is useful to introduce a more general mathematical definition of the activation energy of desorption

$$E_{des} = -R \frac{d \ln k}{d(1/T)} = RT^2 \frac{d \ln k}{dT} . \tag{4.53}$$

Frequently it is found that Eq. (4.53) obeys the form

$$E_{des} = E_{0,des}^{qm} + mRT . \tag{4.54}$$

p. 185 "The coverage at time t is given by integrating Eq. (4.61) (see also Exercise 4.2)

$$d\sigma = s(\sigma)d\varepsilon = s(\sigma)Z_W \, dt \tag{4.63}$$

where ε is the **exposure**. The coverage is linearly proportional to the exposure only if the sticking coefficient is constant as a function of coverage, which is often true at very low coverage, for metal on metal adsorption or condensation onto multilayer films."

p. 197–198 "First-order desorption leads to asymmetric peaks. Second-order desorption leads to symmetric peaks."

p. 199 In Fig 4.14(d), the simulations have been properly calculated but have been labelled in reverse order. They should appear as they do below.
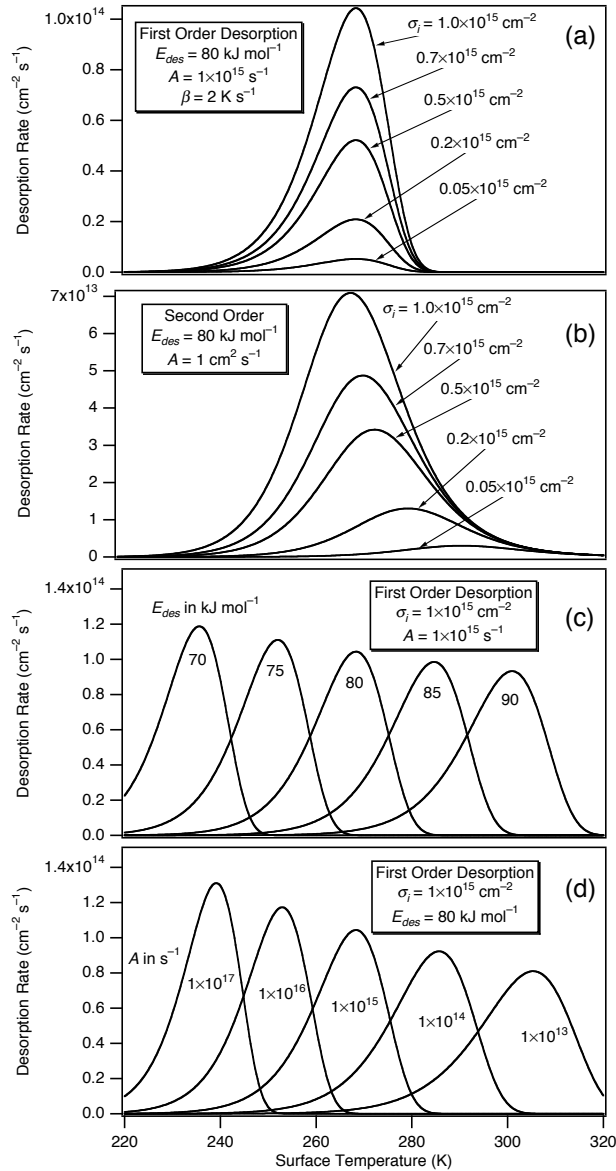
Fig. 4.14

p. 203

4.6 Consider precursor mediated adsorption through an equilibrated precursor state. The activation barrier to desorption out of the precursor is E_{des} and the activation barrier separating the precursor from the chemisorbed state is E_a. Prove mathematically that in precursor mediated adsorption, if $E_{des} > E_a$, increasing the surface temperature decreases the sticking coefficient and if $E_{des} < E_a$, increasing T_s favours sticking.

p. 204

4.14. Write out expressions of Eq. (4.79) in the limits of

Note: Correction to text in which Eq. (4.80) was mentioned)

Chapter 5

p. 225 The final sentence of the second paragraph should read
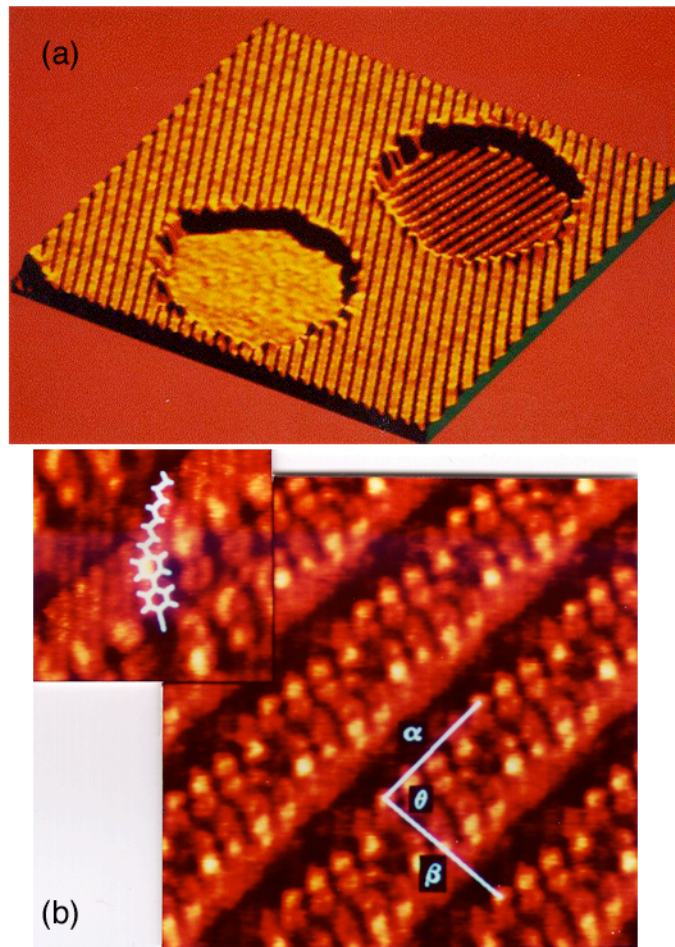
The general composition consists of rhodium, platinum and palladium dispersed on Al_2O_3 with CeO_2 added as a type of promoter.

p. 237 second line should read
 "A Si(100) surface with the same..."

Chapter 6

p. 280 Fig. 6.15. Panel (a) is incorrect but then you can't see it anyway.