

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

Acknowledgements

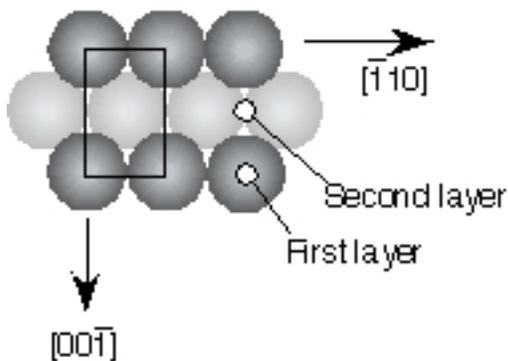
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Chapter 1

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 known as a **depletion layer**.

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



(c) fcc(110)

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

Chapter 2

p. 48 Eqs. (2.21) and (2.22) should have a -1 in the numerator.

$$m_{12} = \frac{-1}{\det \mathbf{M}^*} m_{21}^* \quad (2.21)$$

$$m_{21} = \frac{-1}{\det \mathbf{M}^*} m_{12}^* \quad (2.22)$$

p. 51. The caption to Fig. 2.16 still contains an error:

(a) $(\sqrt{3} \times \sqrt{3})R30^\circ$ (c) (i) fcc(100)–(2×2)

Fig. 2.7 Reproduced with permission from R. Becker and R. Wolkow, *Semiconductor Surfaces: Silicon*, in *Scanning Tunnelling Microscopy* (Eds.: J. A. Stroscio, W. J. Kaiser), Academic Press, Boston, **1993**, p. 193. (c) 1993 Academic Press

Chapter 3

In Exercise 3.14, typo in book reads S_d instead of s_0 .

Fig. 3.12 The interaction strength of chemisorbed O and how it varies across a row of transition metals. In the upper panel, the good agreement between experimental and theoretical results is shown. In the lower panel, the linear relationship between interaction strength and the d band centre is demonstrated. Source of data for experimental results: I. Toyoshima, G. A. Somorjai, *Catal. Rev – Sci. Eng.*, **19** (1979) 105. Reprinted with permission from B. Hammer and J.K. Nørskov, *Theoretical surface science and catalysis – Calculations and concepts*, *Adv. Catal.*, Vol. 45 (Eds.: B. C. Gates, H. Knözinger), Academic Press, Boston, **2000**, p. 71. (c) 2000 Academic Press.

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 [35], that the activation energy, in this case E_{des} , is given by the difference between the mean energy of the reactants $\langle E \rangle_{\text{R}}$ and the mean energy of the molecules in the **transition state** $\langle E \rangle_{\ddagger}$

$$E_{\text{des}} = \langle E \rangle_{\text{R}} - \langle E \rangle_{\ddagger} \quad (4.4.28)$$

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

$$E_{\text{des}} = -R \frac{d \ln k}{d(1/T)} = RT^2 \frac{d \ln k}{dT}. \quad (4.4.29)$$

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

$$E_{\text{des}} = E_{0,\text{des}}^{\text{qm}} + mRT. \quad (4.4.30)$$

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

$$d\sigma = s(\sigma) d\varepsilon = s(\sigma) Z_w dt \quad (4.63)$$

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. 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 $E_{\text{des}} > E_a$, increasing the surface temperature decreases the sticking coefficient and if $E_{\text{des}} < E_a$, increasing T_s favours sticking.

Chapter 6

p. 250, line 8

A tensile force pulls away from the interface.

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

