

## 3.4.2 Adsorption of C, N, and O on metal surfaces

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### 3.4.2.1 Introduction

#### 3.4.2.1.1 General remarks

I would like to start with some general remarks about the completeness of the data presented in this chapter. The amount of data reported in the literature about the properties of adsorbed O, N, and C layers on metal surfaces is hardly tractable on a reasonable time scale, so that the present chapter is inevitably incomplete. This is particularly the case for the electronic properties for which a last comprehensive compilation of data goes back to 1982 [82W1]. The presented tables should rather serve as a first introduction into the wealth of literature about this topic from which the reader may start a more exhaustive literature research. General trends and properties of the adsorbates O, N, and C among the metal surfaces precede each subsection.

#### 3.4.2.1.2 List of acronyms

Acronym	Explanation
AES	Auger-electron spectroscopy
APS	appearance potential spectroscopy
ARPES	angle-resolved photoemission spectroscopy.
ARSIMS	angle resolved secondary ion mass spectrometry
ARUPS	angle-resolved ultraviolet photoemission spectroscopy
b	bulk
BE	binding energy
c.t. 1O	coordinated to one O atom
CEM	corrected effective medium calculations
Cluster	cluster calculations
Cluster	cluster calculations (in contrast to slab calculations)
DFT	density functional theory calculations
DFT-GGA	DFT-generalized gradient approximation
disp.	dispersion
DLEED	diffuse low energy electron diffraction
E(E)LS	electron (energy) loss spectroscopy.
$E_{\text{act}}$	activation energy
EELFS	electron energy loss fine structure
EELS	electron energy loss spectroscopy
$E_i$	impact energy of the incident molecule beam
ELS	electron loss spectroscopy.
EMT	effective medium theory
ESS	equilibrium segregation study
EXAFS	extended X-Ray absorption fine structure
EXELFS	extended electron energy loss fine structure
expos.	exposure
FES	forward-electron scattering.
FFAK	forward focusing of Auger and Kikuchi electrons
FLAPW	full potential linearized augmented plane wave method
FP-LAPW	full potential linear augmented plane wave method
HeD	He diffraction
HEIS	high energy ion scattering

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HRCLS	high resolution core level shifts
HREELS	high resolution energy electron loss spectroscopy
ICISS	impact-collision ion scattering spectroscopy
ID	isothermal desorption
IHA	isosteric heat of adsorption
IPE	inverse photoemission: energies given in eV above $E_F$
IPES	inverse photoemission spectroscopy
ISS	ion scattering spectroscopy
KRIPES	$k$ -resolved inverse photoemission spectroscopy
KW	King Wells method [74K1]
L	gas exposure in Langmuir (1 L = $1.33 \cdot 10^{-6}$ mbar s)
LEED	low energy electron diffraction
LEIS	low energy ion scattering
LT phase	low temperature phase
MCS	Monte-Carlo simulations
MC	micro calorimetry
MDS	metastable deexcitation spectroscopy.
MEIS	middle energy Ion scattering
ML	monolayer
Mol. Beam:	molecular beam according to the King-Wells method
MR	missing row reconstruction
MS	meta-stable phase
NDRS	negative direct recoil spectroscopy
NRA	nuclear resonance analysis
$\nu_D$	frequency factor
PES	photoemission spectroscopy
PhD	photoelectron diffraction
Raman	Raman spectroscopy
RBS	Rutherford backscattering spectroscopy
REM	raster electron microscope
RHEED	reflected high energy electron diffraction
RT	room temperature
SCL	surface core level
SC-LAPW	self consistent linearized augmented plane-wave method
SCLS	surface core level shift
SERS	surface enhanced Raman scattering
SEXAFS	surface extended X-ray-absorption fine structure
SIMS	secondary ion mass spectroscopy
SPALEED	spot profile analyzing LEED
SSXA	surface soft-X-ray absorption
STM	scanning tunneling microscopy
STM-LES	STM-light emission spectroscopy
sub	substitutional
subs.	subsurface
SXES	soft-X-ray emission spectroscopy
SXRD	surface X-ray diffraction
SXW	standing X-ray wave
$T_c$	critical temperature (order-disorder transition)
TDS	thermal desorption spectroscopy
TEAS	thermal energy atom scattering
TOF-SARS	time-of-flight scattering and recoiling spectrometry.
UHV	ultra high vacuum

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UPS	ultraviolet photoemission spectroscopy
XAS	X-ray absorption spectroscopy
XPD	X-ray photoelectron diffraction
XPS	X-ray photoemission spectroscopy
$\Delta\phi$	workfunction change

### 3.4.2.2 Oxygen adsorption on metal surfaces

Sources of oxygen used in UHV experiments are molecular oxygen O<sub>2</sub> (the most frequently used source), nitrogen oxides N<sub>2</sub>O and NO<sub>2</sub>, atomic O (produced by glow discharge plasma) and ozone O<sub>3</sub>. These latter three sources are used to produce high-O-coverages even under UHV conditions. Care has to be taken since NO<sub>2</sub> and O<sub>3</sub> are strongly oxidizing agents which attack even the gaskets of the UHV chamber and the oil in the back pumping system.

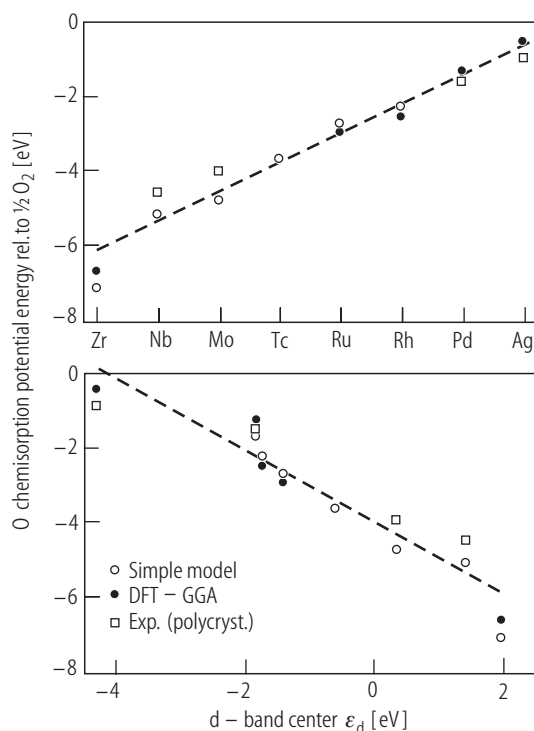
The interplay of chemisorption, subsurface diffusion and oxidation governs the transformation from a metallic to an oxide material and can be monitored with surface sensitive methods. The most weakly bound oxygen species on metal surfaces is the physisorbed oxygen. This kind of oxygen reveals structural, vibrational and electronic properties that are very close to those of gaseous oxygen. On the other hand, chemisorbed molecular oxygen (superoxo- and peroxy species) is bound by about 0.7-1.0 eV, as observed for instance on Pt(111) [98N3] (and references therein) and Ag(110) [96G1] (and references therein). In this section we concentrate on the properties of chemisorbed (atomic) oxygen on metal surfaces.

Chemisorbed (atomic) oxygen needs dissociation of molecular oxygen prior to the adsorption (for dissociative sticking coefficient see Table 1), establishing a strong bond between the atomic oxygen species and the metal surface (see Tables 2 and 3). Details about the adsorption of molecular oxygen on metal surfaces can be found in section 3.7.2. In general the bond strength of chemisorbed atomic oxygen on the metal surface is substantially higher than the binding energy of oxygen in corresponding metal oxides; typical values for chemisorbed oxygen are 5 - 10 eV. Typical experiments in surface science (UHV conditions) are far from thermal equilibrium with the surrounding gas phase. The following scenario is therefore typical for UHV experiments. Beyond a critical coverage of on-surface oxygen, the binding energy of oxygen on the surface is lower than of oxygen accommodated in the selvedge region of the metal surface. Consequently O penetrates into the subsurface region or even dissolves into the bulk for energy reasons. Finally, oxide formation takes place on the metal surface.

Oxygen adsorption on metal surfaces plays a crucial role in the oxidation reaction of molecules over metal catalysts (such as the CO oxidation reaction and the partial oxidation of organic molecules) whose efficiency varies widely with the oxygen coverage on the surface. This variation in catalytic activity is attributed to the dependence of the oxygen adsorption energy which determines predominantly the activation barrier for simple oxidation reactions. In turn, the binding energy of oxygen to the underlying catalyst surface is a function of the mutual interaction among the adsorbed O atoms and depends on the actual configuration of the surface [79E2, 77B7, 81S2, 98O1]. For instance, beyond a critical coverage several metal surfaces allow O penetration and diffusion into the bulk region which eventually may result in the formation of a metal oxide. There are some (rare) exceptions from this general tendency: For Zr, Ti and Ta subsurface O is more stable than on-surface oxygen. These variations in the binding energy of oxygen affect directly the catalytic activity.

Catalysis by transition-metal surfaces exhibits characteristic trends across the periodic table whereby metals that form chemical bonds of intermediate strength have the highest activity. The strength of the O-metal bonding is frequently related to its propensity to dissociate molecular oxygen on metal surface. For instance the O-Ag bonding is much weaker than on Ru or Ti, and also the dissociative sticking coefficient is much smaller on Ag than on Ru or Ti (see Table 1). An exception to this general rule is aluminum: Although the O-Al bonding is strong, dissociative sticking is very low (see Table 1). The reason is that the missing d-electron density of Al does not allow for high dissociation probability while the s-electron density causes a strong bonding. For a more thorough discussion of this effect, the reader is referred to [95J1]. Norskov et al explain the binding energy of oxygen among the transition metals to be related to

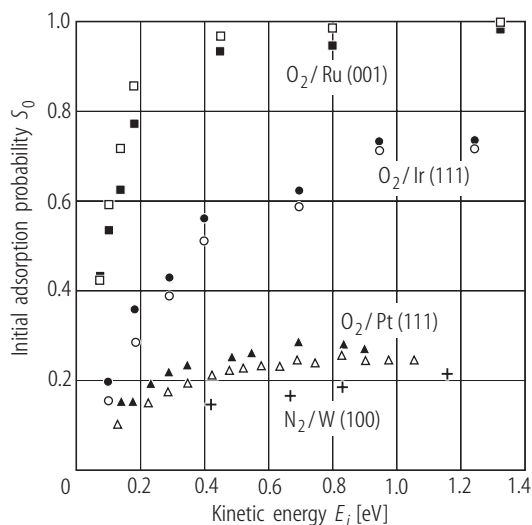
the position of the d-band center (see Fig. 1). To reach high activity on metal surfaces, a low O-metal bonding has to be balanced against the simultaneous reduction in the dissociative sticking probability. This is accomplished with transition metals that bind atomic oxygen moderately strong (so called Sabatier Principle).



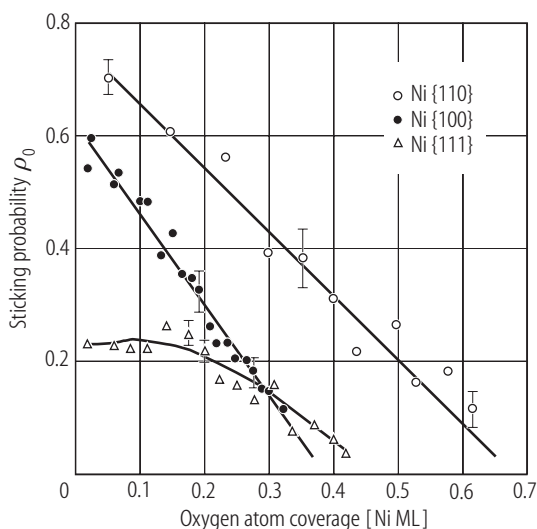
**Fig. 1.** Calculated and experimental values of the binding energy of adsorbed O atoms on various transition metals are indicated along the 5th row in the Periodic Table. Also shown are the O binding energies as a function of the energetic position of the d-band center; [00H1].

Molecular beam techniques have become a powerful tool to study the dynamics of dissociative chemisorption of molecules, such as oxygen, on well-characterized single crystalline surfaces in UHV (see Table 1). The advantage of using molecular beams is that kinetic and vibrational energy of the impinging gas molecules are well-defined and can be controlled. Many of these investigations have indicated that dissociative chemisorption occurs mainly through two different mechanisms: a direct dissociative mechanism and a precursor-mediated mechanism [97D2]. If the translational energy of the incident O<sub>2</sub> molecule promotes the dissociative chemisorption of a molecule at a surface then such a mechanism has been termed direct dissociation. However, it is also possible that kinetic energy may assist in surmounting barriers to molecularly chemisorbed surface states as well (a direct molecular chemisorption mechanism) which then serve as precursors to dissociation. According to [97D2] the general trend is as follows: Systems demonstrating molecularly chemisorbed states which are stable at low temperatures and coverages appear most consistent with dissociation mechanisms involving direct molecular chemisorption for incident energies up to few electron volts. These molecular states have been identified by HREELS and NEXAFS (see for example 98N2).

Specific values for the dissociative sticking coefficient and other details about the dissociation process are compiled in Table 1. In general, the dissociative sticking coefficient depends strongly on the impact energy of the incident O<sub>2</sub> molecules. This property is illustrated in Fig. 2 for various close-packed metal surfaces. In Fig. 3 we show an example for the dissociative sticking coefficient of O<sub>2</sub> on various orientations of Ni as a function of the adsorbed O coverage [97S1].



**Fig. 2.** Measurements of the initial adsorption probability  $S_0$  versus kinetic energy  $E_i$  for  $O_2$  on Ru(001) (filled squares: 77 K, open squares: 500 K); for  $O_2$  on Ir(111) (filled discs: 77 K, open discs: 425 K); for  $O_2$  on Pt(111) (filled triangles: 200 K, open triangles: 350 K); and for  $N_2$  on W(100) at 300 K; [97D2].

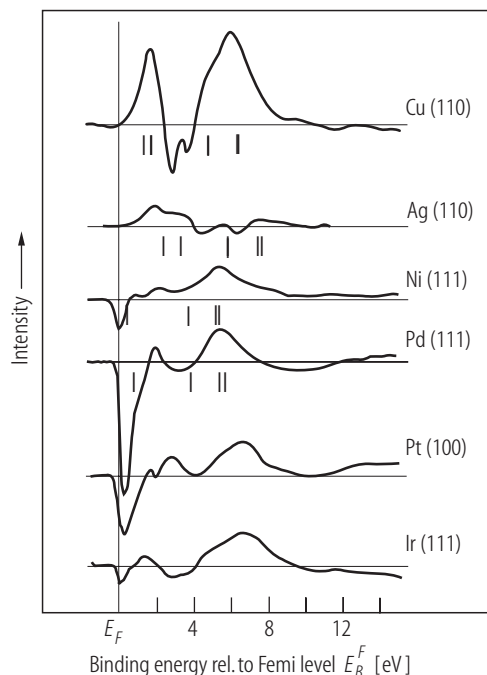


**Fig. 3.** Dissociative oxygen sticking probability on Ni{100}, Ni{110} and Ni{111} at 300 K in the low O-coverage region; [97S1]. A thermal molecular beam at room temperature was used.

Other experiments, which do not use molecular beam techniques, introduce the  $O_2$  gas through a leak valve. The introduced oxygen gas is at room temperature with a Maxwellian energy distribution for the kinetic energy. Thus the experimental value for the dissociative sticking probability provides an energy averaged value. In general, these values are closer to the reality in catalytic reactions than those obtain by molecular beam experiments.

The binding of O atoms to metal surfaces is prevalently covalent. It encompasses two contributions, one is coming from the coupling of O(2p) to the metal s states, and the other is due to the extra coupling to the d-states. Since the contribution from the metal s states to the O-metal bonding is approximately the same for all late transition metals, the main trends in the chemisorption energy is given by the interaction with d electrons (see Fig. 1). The coupling of the localized d states gives rise to a bonding and an anti-bonding state (tight binding argument). As we move from Cu, Ag, or Au to the left in the Periodic Table, the d-bands move up in energy, and progressively more anti-bonding adsorbate-metal d states become empty. For Cu, Ag, and Au the anti-bonding states are completely filled because the d-bands are well below the Fermi level. The variation in the adsorption strength from Cu, Ag, and Au is determined by the Pauli repulsion between O(2p) and the completely filled d-states. Au has the most extended d states, and therefore the strongest repulsion. This explains why Au is the noblest metal among Cu, Ag, and Au [95H2]. With oxygen in metal oxides the contribution of ionic bonding becomes more important than in the chemisorbed phase of oxygen on metal surfaces.

The chemisorbed O species is mostly covalently bound to metal surfaces, as characterized by typical XPS values of O(1s) appearing at 531.5 eV. In the valence band region, the peaks characteristic for atomic oxygen are located at about 6.5 eV below the Fermi level ( $E_F$ ) (see Table 4). This energy position for the O(2p) derived emission from adsorbed atomic oxygen is typical for most transition metals [78K1]. The emission of molecular surface oxygen is centered at 8 eV below  $E_F$  and has a remarkable width (FWHM) of 4.5 eV.



**Fig. 4.** Angle-integrated UPS Spectra ( $h\nu = 40.8$  eV) from various oxygen covered transition metal surfaces. The spectrum for Ag(110) originates from the work by Bradshaw et al. [74B1], while all other spectra are taken from the work by Küppers and Ertl [78K1]. The bars under the spectra denote one-electron multiplet energies as calculated by Doyen and Ertl [78D1]. The presentation is taken from [82W1]. O(2p) derived emission appears at about 6 eV.

In Fig. 4, we show angle-integrated UPS spectra from various oxygen covered transition metal surfaces. ARUPS data have established the energetic splitting of both levels into O(2p<sub>z</sub>) derived  $\sigma$ ,  $\sigma^*$  and O(2p<sub>x,y</sub>) derived  $\pi$ ,  $\pi^*$  states. On transition metals with high density of d-states at  $E_F$  only the bonding molecular orbitals (MO) are filled and show up in UPS, whereas the anti-bonding MO's are located above  $E_F$  and are empty. As shown by Hammer and Norskov [00H1] this MO scheme with bonding and anti-bonding orbitals is of general validity for the oxygen-metal chemisorption bond.

Subsequent oxygen incorporation and incipient oxidation is accompanied by a substantial redistribution of the valence band emission. The O(1s) emission changes from 531.5 eV to 529.5 eV, which is largely independent of the substrate metal [82W1]. In the chemisorbed oxygen phases on metal surface, the surface core level shifts of the metal atoms are linearly related to the number of O atoms coordinated to it, see for example the systems O-W(110) [98R1] and O-Ru(0001) [01O1]. Typically, the core levels of surface metal atoms shift to lower values with increasing O-coordination (see Table 4 and compare also section 4.3).

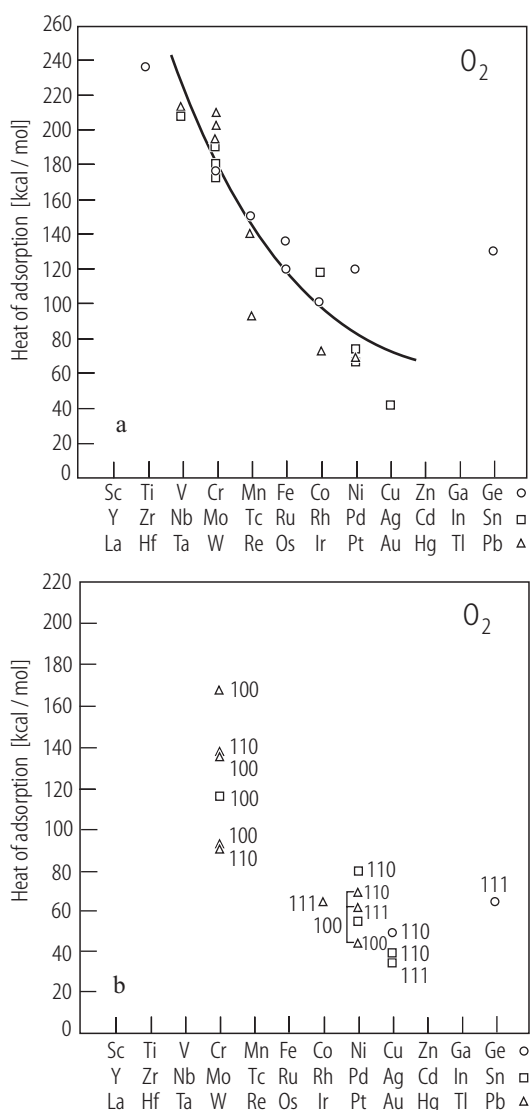
The oxygen against metal vibrations are in the energy range of 40 meV to 90 meV, a typically value is 60 meV (see Table 5).

The local adsorption geometry of oxygen on metal surface (see Table 6) can roughly be divided into non-reconstructive adsorption, which frequently occurs on low-index surfaces, and reconstructive adsorption. The adsorption site found for oxygen is in good agreement with the general tendency that adsorption of chalcogen atoms on high density transition metal surfaces takes place at those adsorption sites with the highest coordination number and also on which an additional metal layer would have grown. Marcus et al. [75M2] advocated first this empirical law.

The general trend of atomic adsorbates to chemisorb in high-coordinated sites was later corroborated by Effective Medium Theory (EMT) considerations. According to this theory, which has been put forward by Nørskov and coworkers [90N2], the actual bonding configuration of the adsorbed oxygen atom is the result of a delicate balance of reaching the optimum electron density offered by the metal substrate surface and minimizing the Pauli repulsion between the metal and the adatom charge density. If the adatom is coordinated to many metal atoms the optimum electron density is provided by a larger bond-lengths that minimizes the Pauli repulsion, and thus making high-coordination adsorption sites favorable.

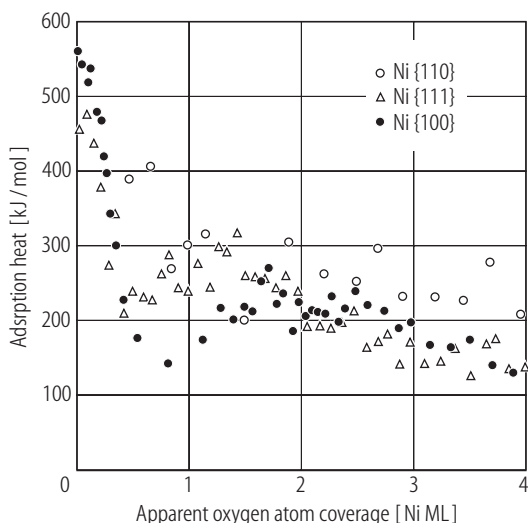
Some early transition metals behave quite differently. With the O-Zr(0001) system we are faced with the interesting situation where only after a critical O coverage is accommodated below the surface, on-surface oxygen becomes stabilized, while for other metal surfaces, a critical on-surface O coverage is needed for the commencement of oxygen penetration into the sub-surface region [95W1, 95W2, 97W1].

In general the heat of adsorption does not vary very much from one surface plane to another [79E3] so that values found for polycrystalline samples serve (at least) as a guideline (see Fig. 5).



**Fig. 5.** (a) Heats of adsorption of  $O_2$  on polycrystalline transition metal surfaces. (b) Heats of adsorption of oxygen on various single crystal surfaces of transition metals; [94S4]. These are TDS data.

In a naive picture one would assume that the strength of the chemisorption bond increases as the number of “unsaturated” valencies of surface atoms increases, i.e. if the coordination number of the metal surface atoms decreases. This would imply a lower adsorption energy at the most densely packed planes compared to planes with higher Miller indices. A more elaborated view was put forward by Hammer and Nørskov [00H1]. From thermal desorption experiments it is known that with increasing O coverage the activation energy for desorption (see Table 2) and therefore the O-metal bonding (see Table 3) weakens as the result of a net repulsion among the O atoms. This observation is exemplified with oxygen adsorption on various orientations of Ni surfaces (see Fig. 6).



**Fig. 6.** Caloric heats of adsorption of O<sub>2</sub> as a function of coverage in the oxide film formation region for all three low index Ni surfaces; [98B2].

Yet the O-metal bond-lengths do not follow this general trend [98O1]. In most of the cases, the O-metal bond-length remains constant or even decreases slightly with increasing O coverage as demonstrated with Ru(0001) and Ni(111). The effective O radii, which are derived from the value for the O-metal bond-length, slightly exceed the covalent radius by 0.1 Å. This is consistent with a comparatively small net charge transfer from the substrate to the oxygen adatom and a prevalently covalent bonding. The effective O radius increases also with the coordination number. Varying the coordination from threefold to fourfold results in an increased O radius of about 0.1 Å (cf. Ni, Pd, and Rh, Table 6). The adsorption energy of oxygen increases only slightly by a few tenth of an eV (see Table 3), when increasing the coordination number, e.g. from three to four, such as with fcc(111) and fcc(100).

It is interesting to note that TD data (as collected in Table 2) are quite difficult to find by a literature research and most of the derived values of the heat of adsorption are not very reliable. The reason is that during the heating ramp of a typical TD experiment not only desorption takes place but also bulk dissolution, phase transition, oxide formation, reaction with other adsorbed species etc.. For instance for aluminum, oxygen desorption is not possible to measure since the O-Al bonding is so strong that Al will melt before O<sub>2</sub> desorption can take place. For hexagonal cobalt oxygen desorption takes place at temperatures where Co transforms from hcp to fcc lattice.

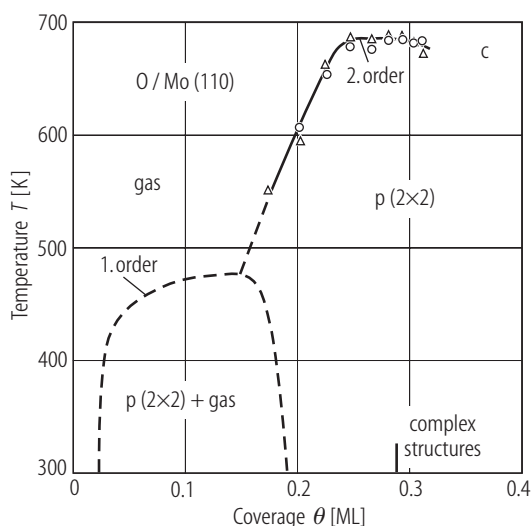
The interaction between O atoms has partly electrostatic origin in that the O induced dipoles interact with each other. The chemisorption-induced dipoles of on-surface oxygen cause in general an increase of the workfunction (see section 4.2), while subsurface O decreases the work function. If O atoms come to close to each other direct orbital overlap may occur, which could lead to O<sub>2</sub> formation with subsequent desorption. Similar to many other chalcogens, oxygen atoms try to prevent a situation where O atoms have to share a common metal atom [98S1].

A very important type of interaction among the O atoms is indirect through their bonds with the metal surface. This interaction exhibits an oscillatory character, i.e. it may be attractive or repulsive depending on the mutual separation. It decays within distances of two to three lattice constants to values below  $kT$ . The indirect interaction is considered to be crucial for the development of ordered oxygen layers on metal surfaces (see Table 7). In order to form ordered overlayers the mobility of the O atoms has to be high

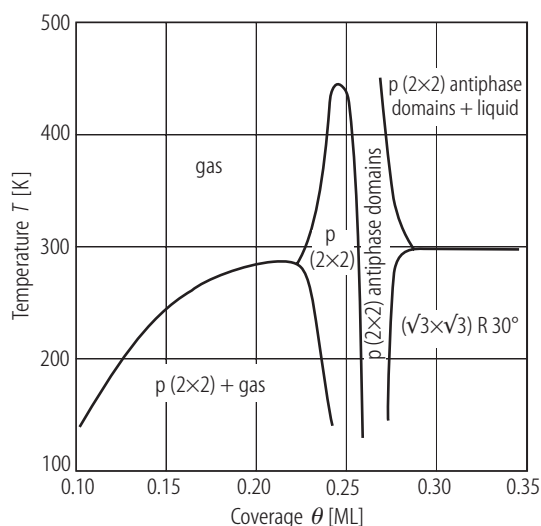


enough to reach the thermodynamical stable configuration. The diffusion barrier determines the mobility of O atoms across the surface. Their values are about one order of magnitude smaller than the strength of the chemisorption bond itself. The interaction among the O atoms in an ordered phase manifests itself in the formation of 2D-band structures, which can be identified for instance with ARUPS even in the case of a (1×1) overlayer. On more open surfaces, such as the fcc(100), disordered O-overlayers are more frequently observed than on densely-packed surfaces, e.g fcc(111). This is presumably due to the higher activation barrier for O diffusion on fcc(100) compared to fcc(111).

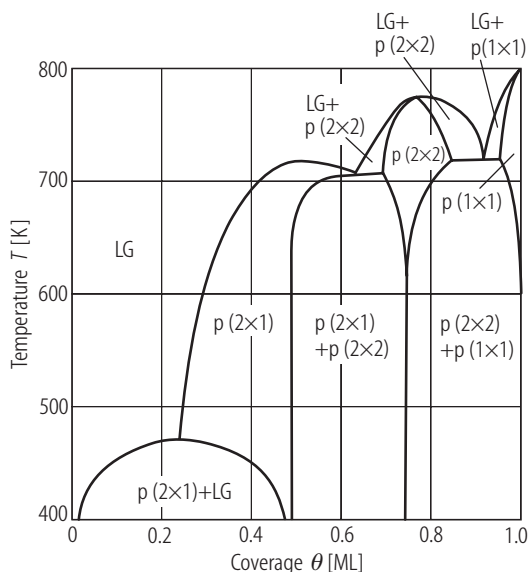
Evidently the energy of the system depends on the mutual configuration of the adsorbed particles and therefore no longer the configuration with maximum entropy (equal to random distribution) will characterize the equilibrium. As a result long-range order may occur, depending on the interaction between the O atoms and the thermal energy  $kT$ . The adsorbate system may be treated with the methods of statistical thermodynamics. At finite temperatures the statistical properties of adsorbate systems may be described by two-dimensional models [76B1], such as the Ising model or the 3-state, 4-state Potts models, leading to an order-disorder transition at a critical temperature (see Table 8). A comprehensive collection of experimental phase diagrams are indicated in Figs. 7 - 10.



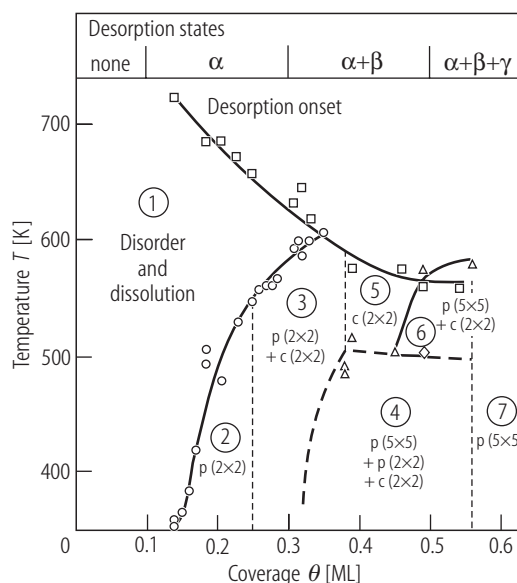
**Fig. 7.** Phase diagram for O-Mo(110); [86W2]. The dashed lines are extrapolations from LEED measurements.



**Fig. 8.** Coverage versus temperature phase diagram for O-Ni(111); [81K1].

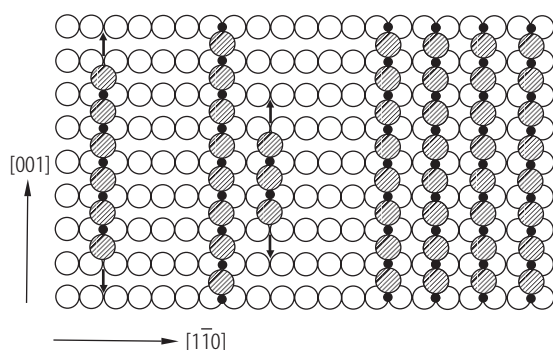


**Fig. 9.** Phase diagram for O-W(110). LG denotes “lattice gas”; [89W2].



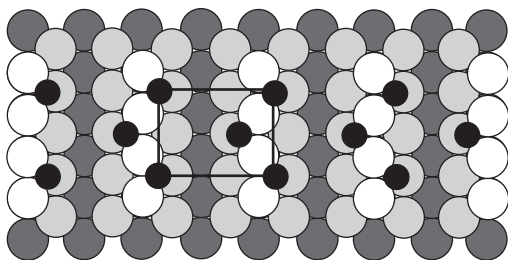
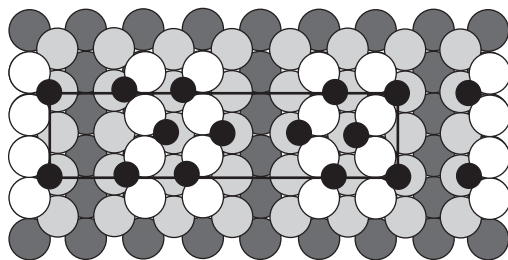
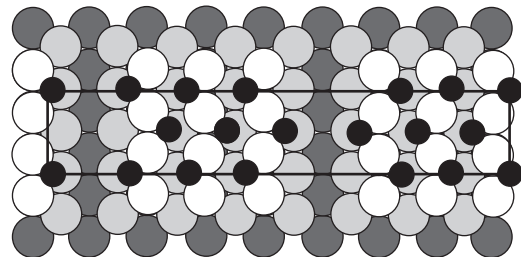
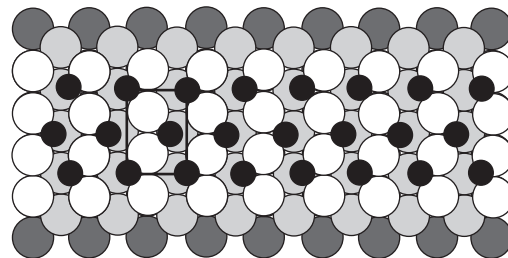
**Fig. 10.** Phase diagram for the system oxygen/Pd(100). Solid lines are used to connect data points; dashed lines are assumed or possible boundaries; [88C1].

Since the chemisorption strength of O on metal surfaces is quite high, the adsorption is accompanied by substantial reconstructions of the metal surface (see section 4.1), either locally [94S3] or with mass transport involved [93B1, 96T1, 98C1]. Prominent examples of the latter class are O-induced added row reconstructions on the fcc(110) surface of Ni, Pt, Rh, Pd, Cu, and Ag. The reconstruction is driven by the prospect to form stronger O-metal bonds; this tendency is facilitated by soft metals, which exhibit relatively weak metal-metal bonding. The added row reconstruction on Cu(110) has been considered as the first step towards oxidation [95L2]. The preference of oxygen to bind to low-coordinated metal atoms was explained in the framework of EMT [90N2]. Thus, oxygen chemisorption in long-bridge sites on a (2×1) added row reconstructed Cu(110) surface [90C2] (see Fig. 11) becomes energetically more favorable than adsorption in the first Cu layer of the unreconstructed surface, which overcompensates even the cost of breaking metal-metal bonds.



**Fig. 11.** The added row (or missing row) structure induced by oxygen adsorption on Cu(110), Ni(110) and Ag(110); [96O2]. The small black balls represent the oxygen atoms. The big hatched and white balls represent the substrate atoms of the first and second substrate layer, respectively. The arrows indicate the growth direction of the metal-O rows.

Note that the coordination of the outermost Cu atoms on the (2×1) missing row reconstructed surface is reduced from six (ideal (110) surface) to four and oxygen in long-bridge sites allows oxygen to bind to two under-coordinated metal atoms.

Rh(110)-(2×2)p2mg-2O,  $\theta = 0.5$ , 1×2 missing rowRh(110)-c(2×6)-8O,  $\theta = 0.67$ , 1×3 missing rowRh(110)-c(2×8)-12O,  $\theta = 0.75$ , 1×4 missing rowRh(110)-(2×1)p2mg-2O,  $\theta = 1.0$ 

**Fig. 12.** The stable O-phases on Rh(110) as they develop with increasing O-coverage. Except the (2×1)p2mg-2O structure, all other phases are characterized by a missing row type reconstruction of the underlying Rh(110) surface; [98O1]. The small black balls represent the oxygen atoms. The big white, grey and dark grey balls represent the substrate atoms of the first, second and third substrate layer, respectively.

On Rh(110) oxygen adsorption induces the (1×n) missing row reconstruction (see Fig. 12), where densely packed Rh-rows are completely missing. Oxygen adsorption proceeds then on the (1×2) troughs in quasi-threefold sites instead of (1×1) troughs. Oxygen atoms are attached to two Rh atoms in the topmost layer and one Rh atom in the second. This site preference is explained by the propensity of oxygen atoms to bind to lower coordinated metal atoms. For steric reasons the oxygen does not form a (n×1) added row reconstruction on Rh(110) because the topmost Rh-Rh separation along the [001] direction is too small to allow the O atoms to be incorporated [98C1].

### 3.4.2.2.1 The dissociative sticking coefficient of oxygen on metal surfaces and its dependence on the impact energy of the incident O<sub>2</sub> molecule, $E_i$

**Table 1.** Sticking coefficient

Substrate	Coverage	Sticking coefficient	Impact energy $E_i$ [eV]	Remarks	Method	Ref.
Ag(110)	initial	0.63		direct molecular chemisorption O <sub>2</sub> (ad) → O(ad)	Mol. beam	94V2
	initial	~1	0.8	molecular adsorption	Mol. beam	94V3
	initial	1.7×10 <sup>-3</sup>		100 K: O <sub>2</sub> (gas) → O(ad)	STM, backfilling	98Z1
		1.9×10 <sup>-3</sup>		500 K: O <sub>2</sub> (gas) → O(ad)		
	initial	2×10 <sup>-4</sup>		477 K	TDS, XPS, LEED	84C2
		10 <sup>-3</sup> - 10 <sup>-2</sup>	0.1	RT		
	initial	0.1 - 0.4	>0.4	RT	Mol. beam	96R2
Ag(111)	initial	10 <sup>-7</sup>	0.1	direct and precursor mediated steps are important	Mol. beam	96R1, 95B3, 97R2, 97R3
		10 <sup>-6</sup>	0.9			
		10 <sup>-3</sup>	1.8			
	0-0.41 ML	10 <sup>-6</sup>		490 K	TDS	85C1
	initial			explain mol. beam of [96R1]	Theory	97Z1
Ag(100)	initial	4.4×10 <sup>-3</sup>	<0.8	no direct dissociation channel, molecular precursor O <sub>2</sub> (ad) → O(ad)	Mol. beam	96B3
		~1	0.8			
		>0.3	>0.5	RT: dissociative sticking sticking probability strongly decreases for $E_i$ < 0.5 eV	Mol. beam	96R2
		8×10 <sup>-4</sup>		$E_{kin} = 88$ meV	Mol. beam	90R3
Al(110)	initial			1.7 × higher than on Al(111)	XPS, AES	79M2, 77M1
	initial	0.04			XPS, AES	84B2
Al(111)	initial	0.0045			STM, backfilling	93B2
	initial	<0.004		on defect free surfaces	HREELS	99Z1
	initial	<0.01	0.030	RT	Mol. beam	97Ö1
	initial	0.9 <sup>a)</sup>	0.6 - 2.0	RT <sup>b)</sup>	Mol. beam	97Ö1
	initial	0.04			Mol. beam	84B2
		0.0053			Ar bombardment	
Al(100)	initial			1.4 × smaller than on Al(110)	XPS	79M2
	initial	0.008			XPS	84B2
Be(0001)	initial	0.1			TDS	84F1

Substrate	Coverage	Sticking coefficient	Impact energy $E_i$ [eV]	Remarks	Method	Ref.
Co (10 $\bar{1}$ 0)	initial	~0.25			$\Delta\Phi$	90S1
Co(0001)	initial	0.3			$\Delta\Phi$	79B1
	initial	0.6		120 K, 300 K	UPS, AES	82C1
fcc-Co(100)	initial	0.8			UPS, AES	77R1
Cr(110)	1/8 ML	0.08		averaged value; sticking coeff. increases with O-cov.	AES	86S3
Cu(110)	initial	0.65	0.050	100 K	Mol. beam, trapping-mediated	93H1
		0.25	0.050	330 K		
		0.8	0.5	330 K		
		a), b)		d); direct dissociation	Mol. beam, Quantum dynamics	93H1, 97D2 96G2
	0.3	0.050				
	0.8	0.8				
Cu(111)	0 - 0.3 ML	0.001		300 K, constant	AES	79H3, 82S4
Cu(001)	initial	0.04	0.050	direct and activated	Mol. beam	93H2
		0.8	0.365			
		a), f)			Mol. beam	99M1
	initial	0.03			XPS, TDS	79H1
	initial	0.02	0.020		Quantum dynamics	96G2
Fe(110)		0.6	0.800			
	initial	0.3	0.050	RT; directly activated for $E_i > 150$ meV, precursor-trapping-dissociation for low surface temperature and low $E_i$ .	Mol. beam	94H2
	c(2 $\times$ 2)O	0.02			backfilling the chamber	80P1
	initial	0.13/0.20			backfilling the chamber	80P1, 76D2
Fe(111)	1 ML O	0.1			AES	00A1
Fe(100)	0.15 ML	0.32			TDS + LEED	84S3
	initial	0.6		extrapolated		
Ir(110)	initial	0.8	0.050	85 - 1000 K	Mol. beam, trapping mediated	95K1
		0.9	>0.5			
Ir(111)	initial	0.2		77 K	Mol. beam, trans. energy 0.10 eV; trapping mediated	97D1
		0.1		425 K		
		0.7	0.8			

Substrate	Coverage	Sticking coefficient	Impact energy $E_i$ [eV]	Remarks	Method	Ref.
Ir(100)-(1×5)	initial	0.10			Mol. beam	98A1
	initial	0.05		425 K	TDS	79K1
Ir(100)-(1×1)	initial	0.24			Mol. beam	98A1
	initial	0.25		425 K	TDS	79K1
Mo(110)	initial	0.50			AES, TDS, LEED	83B2
	0.33 ML	0.10				
stepped (110)	initial	~0.70		step distance 25 Å		
Mo(111)	initial	~1.0		sticking coeff. is constant	XPS	85M1
Mo(100)	0 - 0.33 ML	1.0			AES, $\Delta\phi$	79B2
	0.33 - 0.5 ML	0.87				
	0.5 - 0.8 ML	0.65				
	0.8 - 1.0 ML	0.50				
Ni(110)	initial	0.23			Mol. beam	97S1
Ni(111)	initial	0.78			Mol. beam	97S1
Ni(100)	initial	0.63			Mol. beam	97S1
	initial	1.0			TDS, LEED	74H1
Pd(110)	initial	0.95		473 K	TDS	99Y2
	0 - 0.3 ML	~0.8		sticking coeff. is fairly constant		
	>0.5 ML	→ 0				
Pd(111)	initial	0.65 → 0.4		100 K → 650 K; Direct molecular chemisorption; physisorbed state is precursor of the chemisorbed molecules and these again are precursors for the dissociated O species; precursor conversion from peroxide to atomic O: Energy barrier 0.32 eV.	Mol. Beam	98S2, 98N1
	initial	0.1			TPD, AES	89G1
	0.05 ML	0.87		300 K		
	0 - 0.25 ML	0			TPD, LEED, UPS	77C2
	initial	0.3				
	initial	0.75		323 K	Mol. beam, STM	01K1
		0.50		623 K		

Substrate	Coverage	Sticking coefficient	Impact energy $E_i$ [eV]	Remarks	Method	Ref.
Pd(100)	0.25 ML	~0.1		300 K, p(2×2): 2 L O <sub>2</sub>	TDS/LEED	93K2
	0.5 ML	~0.003		300 K; c(2×2): 180 L O <sub>2</sub>		
Pt(110)-(2×1)	initial	0.3		300 K	TDS, AES	86F1
	initial	0.4		300 K	TDS, AES	76D1
	initial	0.55		170 K	TDS, AES	98W2
		0.42		300 K		
		0.24		600 K		
	>0.25 ML	0.03				
Pt(111)	initial	0.3	0.05	200 K	Mol. beam, precursor mediated	91R1, 88L1
	initial	0.1	0.05	350 K	Mol. beam, precursor mediated	91R1
	initial	a), c)		e); direct molecular chemisorption	TDS, XPS	78N1
	initial	0.2			TDS, XPS	73B2, 77H2, 81C1
Pt(100)-hex	initial	<0.003			Mol. beam	84N1, 94G2
		a), b), c), f)		mechanism ambiguous	Mol. beam	97D2
Pt(100)-(1×1)	initial	>0.20			Mol. beam, precursor mediated	84N1, 96B2
Re (10 $\bar{1}$ 0)	0 - 0.5 ML	0.53		stick. coeff. constant and decreases then rapidly ( $T = 353$ K)		79P1
Rh(110)	initial	0.7		125 K sample temperature	AES, LEED	92C4
	initial	0.95		258 K, 573 K sample temp.	TDS, LEED	90S2
Rh(111)	initial	~0.5		100 K; assuming saturation at 0.5 ML	TPD, AES	85M2
	initial	0.6		110 K - 150 K	Mol. beam	97B3
Rh(100)	initial	0.74		300 K	Mol. beam	98K1
	>0.5 ML	0.04				
	<0.8 ML	0.8		100 K; stick. coeff. constant; partially molecular	XPS, LEED, TDS	83F2
Ru (10 $\bar{1}$ 0)	<0.5 ML	0.4			LEED, TDS	77K1, 96R1
	>0.5 ML	0.24				
Ru(0001)	initial	0.3	0.050	77 - 500 K	Mol. beam, trapping mediated	96W3
		0.95	>0.2			
		a), b), c), f)		d); direct dissociation		

Substrate	Coverage	Sticking coefficient	Impact energy $E_i$ [eV]	Remarks	Method	Ref.
V(111)	initial	0.95	0.045		Mol. beam, direct chemisorption	00B2
		0.58	0.160			
	0 - 0.3 ML	0.75	0.085			
V(100)	(1×5)O	0.40		473 K	AES	01S1
		0.60		873 K	KW	
W(110)	initial	0.28			AES, TDS, LEED	77B4
	initial	0.38			AES, TDS, LEED	80M1
	initial	0.55		300 K	SCLS, UPS O(2p)	98R1, 79W2
		0.35		1000 K		
	initial	0.43		300 - 1350 K	TDS	75E1
	0.33 ML	0.19			AES, TDS, LEED	77B4, 80M1
	0.5 ML	0.05			SCS, UPS O(2p)	98R1
	0 - 0.5 ML	0.2 - 1.0 <sup>a), b)</sup>		d); typical values; direct dissociation	Mol. beam	86R3
W(100)	0 - 0.25 ML	1.0		300 K	TDS, AES	76B3, 79W2
		1.0		1050 K		
	0.25 - 0.5 ML	1.0		300 K		
		0.73		1050 K		
	0.5 - 0.75 ML	0.39		300 K		
		0.44		1050 K		
	0.75 - 1.0 ML	0.24		300 K		
		0.24		1050 K		
	0.0 - 1.0 ML	0.98 - 0.05		linearly	TDS, AES	72M1
Zr(10 $\bar{1}$ 0)	<0.5 ML	1		for $T$ = 90, 293, 473 K up to 0.5 ML; stick. coeff. remains even high during oxidation	LEED, NRA, AES	94Z1

a) =Initial adsorption probability increases with increasing kinetic energy

a') =Initial adsorption probability decreases with increasing kinetic energy

b) =Initial adsorption probability scales with normal kinetic energy

c) = Initial adsorption probability is surface temperature dependent

d) = Saturation coverage is kinetic energy dependent.

e) = Molecular intermediates detected after high kinetic energy exposure

f) = Initial adsorption probability increases with increasing surface temperature

f') = Initial adsorption probability decreases with increasing surface temperature

g) = No surface temperature dependence observed between 300 and 1000 K



### 3.4.2.2.2 The heat of adsorption of chemisorbed oxygen overlayers on metal surfaces

**Table 2.** Heat of adsorption.

substrate	surface	heat of adsorption/ activation barrier for desorption	Ref./method
Ag(110)	initial	335 kJ/mol	76E1
	initial	173±5 kJ/mol	80B1, 96R2/TDS
	(8×1)O, (6×1)O, (4×1)O	163 kJ/mol w.r.t. O <sub>2</sub>	95C1/TDS
	(2×1)O	180 kJ/mol	99C1/TDS
Ag(111)	(4×4)4O	259±16 kJ/mol	96R1/TDS
poly-Al	initial	820 - 880 kJ/mol	60B1
Co(10 $\bar{1}$ 0) Co(0001)		No O <sub>2</sub> TDS available, due to phase transition of hcp-Co to fcc-Co	01S2
poly-Co	initial	420 kJ/mol	66B1
poly-Cr	initial	727 kJ/mol	60B1
Cu(110)	c(2×6): 0.8ML	Annealing to 800 K: removes 0.3 ML O	87M1
poly-Cu	initial	459 kJ/mol	69M1
Fe(110)	Variable O cov.	No desorption of O <sub>2</sub> up to 1050 K	90S3/TDS
poly-Fe	initial	490 kJ/mol	92G2
Ir(111)		(272 – 41.8 $\theta$ ) kJ/mol	76I1/TDS
poly-Mn	initial	635 kJ/mol	60B1/TDS
poly-Mo	initial	802 kJ/mol	66B1/TDS
poly-Nb	initial	869 kJ/mol	60B1/TDS
Ni(110)	initial	498±5 kJ/mol	93A2/MC
	initial	605 kJ/mol	91B3/MC
Ni(111)	initial	440 - 470±15 kJ/mol	93A2/MC
Ni(100)	initial	532±5 kJ/mol, that decreases rapidly with coverage	93A2/MC
poly-Ni	initial	300 - 481 kJ/mol	60W1, 60B1
Pd(110)	initial	188 kJ/mol (activation energy)	99Y2/TDS
	c(2×4)	230 kJ/mol	99Y2/TDS
Pd(111)	initial	222 kJ/mol	89G1/TDS
		230 kJ/mol	77C2/TDS
	0.25 ML	800 K TD peak	90B1/TDS
	>1.2 ML	750 K TD peak	90B1/TDS
Pd(100)	initial	160 kJ/mol	88C1/TDS
	initial	130 kJ/mol	93K2
	$\theta$ = 0.5 - 0.8	(173+34 $\theta$ ) kJ/mol,	93K2
poly-Pd	initial	280 kJ/mol	60B1
Pt(110) (2×1)	initial	360 kJ/mol	96W2/MC
	>0.6 ML	170 kJ/mol	96W2/MC
	desorption	860 K → 775 K	77W2/TDS

substrate	surface	heat of adsorption/ activation barrier for desorption	Ref./method
Pt(111)		213 - 176 kJ/mol	81C1
	0.75 ML	4 desorption states at 800, 720, 690, 570 K	89P1/TDS
	0→0.75 ML	184 kJ/mol → 110 kJ/mol	89P1/TDS
		BE = 3.26 → 2.5 eV	
	0 → 0.25 ML	192 kJ/mol → 154 kJ/mol	81C1
	0.04 → 0.25 ML	232±36 kJ/mol	84D1/IHA
	0 → saturation	208 kJ/mol – 13.5 kJ/mol· $\theta/\theta_{\text{sat}}$	99K1/TDS
Pt(100)	(3×1), >0.3 ML	260 kJ/mol	84G3/ID
	0.13 - 0.27 ML	160 kJ/mol, (3×1) → hex	84N1/ID
poly-Pt	initial	288 - 301 kJ/mol	60B1
Rh(110)		Several desorption states: $\beta_1$ – $\beta_5$	90S1/ TDS (10 K/s)
		$\beta_5$ (1150 K) 294±35 kJ/mol,	
		$\beta_4$ (1095 K) 280±10 kJ/mol,	
		$\beta_3$ (909 K) 234±10 kJ/mol,	
		$\beta_2$ (835 K) 215±10 kJ/mol,	
		$\beta_1$ (797 K) 205±10 kJ/mol	
	(2×2)O, 0.5 ML	300 kJ/mol, Rh-O binding: 395 kJ/mol	92C4/TDS
	c(2×8)O, 0.95 ML	205 kJ/mol, Rh-O binding: 348 kJ/mol	92C4/TDS
Rh(111)		Desorption state $\beta$	79T1/TDS (24 K/s)
		$\beta$ (1200 K) 235±10 kJ/mol	
		$\beta$ (700 K, 900 K) 235±10 kJ/mol	95P1/TDS (27 K/s)
		355 kJ/mol	83R1
Rh(001)	initial	386 kJ/mol	98K1/ MC
	$\beta_1$ (1250 K)	360 kJ/mol	83F2/TDS (8.5 K/s)
	$\beta_2$ (920 K)	260 kJ/mol	
	$\beta_3$ (820 K)	210 kJ/mol	
	>0.6 ML	110 kJ/mol	
			98K1/MC
poly-Rh	initial	486 kJ/mol	60B1
Ru(0001)	(2×2)O	400 kJ/mol	85S2
	(2×1)O	315 kJ/mol	
poly-Ta	initial	886 kJ/mol	60B1
poly-Ti	initial	986 kJ/mol	60B1
W(110)	0.1 ML	965 kJ/mol	75E1/TDS
	0 - 1 ML	656 kJ/mol - 482 kJ/mol	75B3/ID
W(111)	0 - 1 ML	627 kJ/mol - 473 kJ/mol	75B3/ID
W(100)	0.25 L O <sub>2</sub>	550 kJ/mol	76B3/TDS
	2.5 L O <sub>2</sub>	492 kJ/mol	76B3/TDS
	0 - 0.3 ML	489 kJ/mol - 579 kJ/mol	75B3/ID
poly-W	initial	878 kJ/mol	66B1
poly-Y	initial	1107 kJ/mol	88C1

Remark:

Adsorption micro calorimetry in surface science studies: The reader can find calorimetrically measured molar heats of adsorption of gaseous adsorbates on wires and ribbons, which are not included in this table [96C2].

### 3.4.2.2.3 Oxygen-metal bond strength (ab initio calculations)

**Table 3.** The O-metal bond strength as computed by *ab-initio* calculations.

substrate	surface	O-metal bond strength	Ref./method
Ag(110)		3.25 eV w.r.t. O	94R1/cluster
Ag(111)	(2×2)O	overlayer: 1.0 eV	00H1/DFT
Ag(100)	initial	3.32 eV w.r.t. O	94R2/cluster
Al(111)	(2×2)O	8.0 eV	95J1
	(1×1)O	8.5 eV, (1×1)O island growth; strong bonding due to O <sub>2</sub> p <sub>x,y</sub>	95J1
	0.25 - 1ML	7.16 eV (2×2)O, 7.32 eV (2×1)O, 7.44 eV (2×2)3O,	01K2/DFT-GGA
		7.63 eV (1×1)O	
Al(100)	initial	7.0 eV	98D3/cluster
Au(111)	(2×2)O	overlayer: -1.0 eV; not stable w.r.t. O <sub>2</sub>	00H1/DFT
Cu(110)	initial	5.20 eV	94R1/cluster
	(2×1)O	2.08 eV	98F2/DFT
Cu(111)	single O	2.84 eV, 3-fold hollow	97L1/cluster
	(2×2)O	overlayer: 2.0 eV	00H1/DFT
	(2×2)O	4.56 eV w.r.t. atomic oxygen	01Z1/DFT
Cu(100)	initial		94R2/cluster
Fe(100)		5.0 eV, Fe-O: 2.57 Å	93B4/cluster
Mg(0001)	(1×1)O	4.35 eV	97B2/DFT
Mo(110)	(2×2)O	O-overlayer: 5.1 eV	00H1/theory
Nb(110)	(2×2)O	5.2 eV	00H1/theory
Ni(111)	(2×2)O	4.77 eV	99H1/DFT
	low cov.	4.98 eV	92S2/cluster
	single O	5.9 eV	97L1/cluster
Ni(100)	(2×2)O	5.03 eV	99H1/DFT
	low cov.	5.60 eV	92S2/cluster
	single O	6.7 eV	93G2/cluster
Pd(110)-(1×2)	(2×2)mgO	4.36 eV (1.26 eV w.r.t O <sub>2</sub> )	02H1/DFT
Pd(111)	(2×2)-O	4.15 eV/3.53 eV	98L1/99H1/DFT
	(√3×√3)-O	4.15 eV	98L1
	c(2×2)-O	3.8 eV	98L1
	(√3×√3)2O	3.6 eV	98L1
	(1×1)O	3.1 eV	98L1
	single O	3.99 eV	97L1/cluster
Pd(100)	(2×2)-O	4.2 eV/3.53 eV	98L1/99H1/DFT
	c(2×2)O	3.8 eV	98L1
	(1×1)O	2.2 eV	98L1
Pt(111)	(2×2)O	2.75 eV	97M1
	(2×2)O	4.26 eV	00L2/DFT
	(2×2)O	5.51 eV w.r.t. O atom; energy diff. hcp-fcc: 0.5 eV	97F2,97F3
	single O	3.14 eV, 2.61 eV	97L1, 97C3/cluster
	single O	2.5 - 2.7 eV	96I1/cluster
	(2×2)O	3.97 eV w.r.t. atomic oxygen	01Z1/DFT-slab

substrate	surface	O-metal bond strength	Ref./method
Pt(100)- (1×1)	0.25 ML	3.80 eV	97G1/DFT-GGA
	0.50 ML	3.0 eV	
	1.0 ML	2.52 eV	
Rh(110)	(2×2)pg	2.75eV	97S6/DFT
Rh(111)	(2×2)O:	5.03 eV, 2.5 eV	98L1, 99G1, 0H1/DFT
	(2×1)O:	4.85 eV (4.93 eV)	
	( $\sqrt{3}\times\sqrt{3}$ )2O	4.6 eV	
	(1×1)O	4.24 eV (4.38 eV)	
	single O	4.61 eV	
Rh(100)	(2×2)-O	5.20 eV, 4.77 eV	98L1/99H1 (DFT)
	c(2×2)O	4.75 eV	
	(1×1)O	3.8 eV	
Ru(10 $\bar{1}$ 0)	c(2×4)-2O:	5.36 eV	98S1/DFT
	(2×1)-2O	5.14 eV	
Ru(0001)	(2×2)O:	5.55 eV, 2.8 eV	96S2, 00H1/DFT
	(2×1)O:	5.28 eV	
	(2×2)3O:	5.06 eV	
	(1×1)O	4.84 eV	
Tc(110)	(2×2)O	overlayer: 3.8 eV	00H1/theory
V(100)	(1×5)O	5.26 eV (0.6 ML) - 5.14 eV (0.8 ML) depending on the O coverage	01K1/DFT
	c(2×2)O	5.18 eV	
Zr(0001)	(2×1)O	10.01 eV/9.0 eV	96Y1/01J1/DFT
	(1×1)O	9.13 eV/8.5 eV	96Y1/01J1/DFT
	(2×2)O	on-surface ads.: 6.5 eV	00H1/DFT

## Remarks:

- Cluster Calculations produce less reliable values for O-metal binding energies than slab calculations.
- Some oxygen binding energies are given w.r.t. atomic O in the gas phase, others are given w.r.t. half of the binding energy of O<sub>2</sub>. Both values differ by about 2.5. eV.

### 3.4.2.2.4 Electronic properties of chemisorbed atomic oxygen

**Table 4.** Electronic properties of chemisorbed atomic oxygen overlayers on metal surfaces.

Substrate	Surface	State	Binding energy [eV]	Remarks	Method	Ref.
Ag(110)	(2×1)O	O(2p)	6	strong dispersion (2 eV) along the Ag-O chains	ARUPS	86P1, 90T1, 97C1
		O(2p) anti-bonding	1.4		theory	76R1, 90T1
		O(1s)	528.1	490 K	XPS	84C2
	(3×1)O, (4×1)O	O(2p) anti-bonding	1.5			97C1
		O(2p <sub>z</sub> )	3.1	weak dispersion of 0.3 eV along Ag chains	ARUPS	98O3
		O(2p) bonding	6 - 8		MDS	92C3
	(2×1)O, (n×1)O	O(2p) anti-bonding	1.5 - 4			
		O(1s)	528.5		XPS	95B5
		O(2p) bonding	9.7		UPS	88S2
	c(6×2)O, c(2×2)	O(2p) anti-bonding	3.1			
		Ag(3d <sub>5/2</sub> )	368.2		XPS	00B1
		Ag(3d <sub>5/2</sub> )	367.7			
Ag(111)	(4×4)O	O(1s)	530.4			77G2, 90R2
		O(1s) bonding	3.8		UPS	
		O(1s) anti-bonding	8.2			
	TD states:	O(β) O(1s)	530.3	chemisorbed	XPS	95B4
		O(β) Ag-3d <sub>5/2</sub>	368.0		XPS	96B5
		O(γ) O(1s)	529.0		XPS	95B4
		O(γ) Ag-3d <sub>5/2</sub>	367.3		XPS	96B5
		O(γ) O(2p)	2.8, 1.8		UPS	96B5
		(4×4)O O(1s)	528.2	oxidic	XPS	85C1, 95B5
Al(110)	25 L -100 L	O(2p)	7 - 8	similar to Al(100)	PES	76M1, 78E1
	100 L	O-induced Al(3p <sub>3/2</sub> ) peaks	73.9, 75.1		PES	78E1
	0.5 L O <sub>2</sub>		74 - 81	chemisorbed O		
Al(111)	(1×1)O (islands)	O(2p <sub>z</sub> )	6.7	strong dispersion of O(2p)	ARPES	79H2, 79E1, 86M1
		O(2p <sub>x,y</sub> )	7.7			
	(1×1)O			band structure	theory	83B4, 82B1
	(1×1)O (islands)	Al(3p <sub>3/2</sub> )	72.5	clean	PES	87M2, 91B2, 93B7
			73	c.t. 1O		
			73.5	c.t. 2O		

Substrate	Surface	State	Binding energy [eV]	Remarks	Method	Ref.
Al(111)			74	c.t. 3O		
cont.	oxide (1×1)O (islands)	Al(3p <sub>3/2</sub> )	75.1		PES	87M2
		O(1s)	532.1	interior	XPS/ theory	91B2
			533.5	perimeter		
	10 L O <sub>2</sub> (1×1)O	O(1s)	74 - 81	anti-bonding Al-O complex (unoccupied state)	SSXA	79B4
			6.7		ARUPS	79E1, 79H2
			7.5	with 0.7 eV dispersion		
	(1×1)O 0.3 ML	O(2p)	5 - 9		SC-FAPW	81W1
		O(1s)	532.1, 535.5			91B2
		Al(2p)	73	clean Al(111): 72.6 eV; small (1×1)O islands: internal and perimeter O atoms		
Al(100)	600 L O <sub>2</sub>	O(KLL)	505		AES	87H2
		Al(L <sub>1</sub> )O(L <sub>22</sub> L <sub>33</sub> )	55			
		Al(2p)	75.3			
			74.3			
	1500 L O <sub>2</sub>	O(1s)	531		XPS	87H2
		O(KLL)	469.8, 484.4, 490.6, 505		AES	87H2
	3 - 100 L O <sub>2</sub>	O(2p <sub>x,y</sub> )	2.5, 7.5	interpretation: O in-plane with topmost Al plane	PES	76Y1, 78E1
					theory	77B6
	100 L O <sub>2</sub>	Al(2p)	75.3, 74.3	anti bonding Al-O complex (unoccupied state)	theory	84B2
					PES	78E1
	(1×1)O	O(2p)	8 - 10		theory	81K3
	10 L O <sub>2</sub>		74 - 81		SSXA	79B4
Co(10 $\bar{1}$ 0)	(2×1)O	O(2p <sub>x</sub> ), O(2p <sub>y</sub> )	6	disperse by less than 0.5 eV		90S1
			7	disperses by 1 eV		
	(2×1)pg-2O	O(2p <sub>x</sub> )	5			90S1
		O(2p <sub>y</sub> )	5.8	disperse by 0.5 eV		
		O(2p <sub>z</sub> )	5.8	disperses by 0.2 eV		
	c(2×4)2O		-1.8, -2.1		IPES	96R3
	(2×1)pg-2O	2 states	-2 - -4		IPES	96R3
	0.5 L, 120 K	O(2p)	2.7, 5.3	O(on-surface)	UPS	82C1
		O(2p)	0.9, 2.8, 5.0, 6.6, 9.3, 11.2	O(bulk)		
	2500 L, 120 K					

Substrate	Surface	State	Binding energy [eV]	Remarks	Method	Ref.
Co(1120)	-	O(2p)	5.5		UPS	95G1
		O(1s)	529.5		XPS	
Cr(110)	c(4×2)O	O(2p)	6.2, 7.4	weak dispersion	ARUPS	88K3
	100 L O <sub>2</sub>	Cr(2p)	574 - 584		XPS	85F1
Cr(111)	<1 L O <sub>2</sub>	O(1s)	529.6		XPS	78G1
		O(2p)	5.5		UPS	
	>1 L O <sub>2</sub>	O(1s)	530.6	oxide	XPS	
Cr(100)	c(2×2)O	O(2p)	6.6	dispersion 0.3 eV	ARUPS	82G1
	(1×1)O	O(2p)	4.9, 6.8	disperse by more than 1 eV		
	100 L O <sub>2</sub>	Cr(2p)	574 - 584		XPS	85F1
Cu(110)	(2×1)O	O(2p) bonding states	5 - 7.8	strong dispersion(2eV) along the Cu-O chains.	ARUPS	84D2, 87C2, 96O1, 97C1
		O(2p) anti-bonding states	1.5		theory	92W1
		Covalent bond: O2p-metal-sp			XAS	89P3
	(2×1)O		-0.2, -0.3	unoccupied single O states	STM-LES	01U1
Cu(111)	500 L O <sub>2</sub> , 100 K	O(1s)	530.5		XPS	90R2
		O(2p)	6.2, 10.1		UPS	82S4, 90R2
		O(1s)	529.8	on-surface	XPS	95D3
		O(1s)	531.3	sub-surface		
	(2√2×√2)R45°	O-Cu: 2p-3d bonding	~6		PES	77T1, 80L1
		anti-bonding	1 - 2			
	(2√2×√2)R45°	O-K emission	525.4	FWHM ≈ 4.2 eV: wide distribution of O(2p)		92W2
	(2√2×√2)R45°	O(2p) derived states	1.4, 6		UPS	77L2, 77T1
	(2√2×√2)R45°	O(2p)	6 - 7	dispersion 1 eV	ARUPS	80L1
	(2√2×√2)R45°			Oxygen K-emission spectra: filled 2p-3d state	SXES	93T1
	low O coverage	O(2p <sub>z</sub> ), O(2p <sub>x,y</sub> ) well separated			SXES, XAS	98W3
Fe(110)	c(2×2)O	O(1s)	530.1		XPS	80P1
	c(3×1)O	O(1s)	530.3		XPS	93S6, 79B3
	c(2×2)O	O-p <sub>x,y</sub> , p <sub>z</sub> -derived	5.5, 7.0		ARUPS	85S3
	c(3×1)O	levels				
	c(2×2)O	O(2p)		dispersion ≈ 0.1 eV	ARUPS	85S3
	c(3×1)O	O(2p)		dispersion ≈ 1.6 eV		
Fe(100)	(1×1)O	O(2p)	7.1, 5.8, 5.0, 4.55		PES	90C1
		O(2p)	-1.7	minority spin polarized	IPE	92H2, 95D2
	(1×1)O	O(p <sub>x</sub> , p <sub>y</sub> )	4.9, 2.2 disp.		ARPES	85P1
		O(p <sub>z</sub> )	6.9, 1.9 disp.			
	(1×1)O	O(2p)	4 - 8	vertical and horizontal bonding	theory	85H1

Substrate	Surface	State	Binding energy [eV]	Remarks	Method	Ref.
Fe(100)	c(2×2)O	O(2p)	5.5, 5.3		UPS	76B1, 77R3
cont.	<3 L O <sub>2</sub>	O(2p)	~6		EELS	84S3
Gd(0001)	0 - 1 L O <sub>2</sub>	O(2p)	5.4, 6.5	chemisorbed O	ARPES	95Z1
	1 - 3 L O <sub>2</sub>	O(2p)	4.8, 5.4, 6.5, 7.6	oxidic-O	ARPES	95Z1
	0.25 L O <sub>2</sub>	Gd(4f)	8.75 → 8.85	surface	PES	96M1
			8.35 → 8.60	bulk oxidic-O		
Ir(110)	oxidic adsorbed O	O(1s)	530.6		XPS	97L2
		O(1s)	528.9			
		Ir(4f <sub>7/2</sub> )	60.7			
Ir(111)		O(2p)	6 - 7		UPS	77C3, 78K1
	expos. <630 K	O(1s)	529.8±0.2	on-surface O	XPS	76Z1
	expos. >650 K	O(1s)	531.5	subsurface O		
Ir(100)	1 - 10 L O <sub>2</sub>	O(2p)	5		UPS	79K1
Mg(10 $\bar{1}$ 0)	1 L O <sub>2</sub>	Mg(2p)	50.79	MgO	PES	89T1
			51.44	O chem.		
Mg(0001)	9 L O <sub>2</sub>		2.9	transition from O-derived 2p to levels of an MgO species.	ELS	81H1, 81N1
				(1×1)O underlayer coexists with MgO	EELS	82F1
	0.5 L O <sub>2</sub>	O(1s)	530.6, 533		XPS	81G1
Mo(110)	(2×2)-1O			Fermisurface mapping: global Peierls distortion induces the (2×2) ordering.		94D1
Mo(111)	low cov.	O(2p)	5.5	HeI	UPS	85M1
			8	HeII		
	100 L O <sub>2</sub>		9.5, 7	HeII		
	0.8 ML		530.6 → 530.2	O(1s)-shift	XPS	
			227.2 → 227.4	Mo(3d)-shift		
Mo(100)	2 - 10 L O <sub>2</sub>	O(2p)	4 - 6		UPS	77W3
Ni(110)	(2×1)O	O(2p <sub>x,y</sub> )	6	strong dispersion of 2 eV along the Ni-O chains.	ARUPS	91P1, 97C1, 96S4
					theory	90N1
	(2×1)O		-3.2			85D1, 85D2
	(3×1)O		-2.0			
	(3×1)O			similar to (2×1)O	ARUPS	96S4
	30 L, 100 K	O(1s)	530	O <sup>2-</sup>	XPS	95R2
			531.5	O <sup>1-</sup>		
Ni(111)	(2×2)O	O(2p)	-1.1 → -2.8	dispersion Covalent bond: O(2p)-metal-sp	IPE XAS	85A1 89P3



Substrate	Surface	State	Binding energy [eV]	Remarks	Method	Ref.
Ni(111) cont.	(2×2)O	Ni(3p <sub>3/2</sub> ) clean	861.5 852	more pronounced at grazing incidence	XPS	76K1
		O(1s)	531.6			
	30 L, 100 K	O(1s)	530	O <sup>2-</sup>	XPS	95R2
			531.5	O <sup>1-</sup>		
	(√3×√3)R30°O	O(2p <sub>z</sub> )	8		PES	79R1, 79C2
Ni(100)	c(2×2)O	O(2p <sub>x,y</sub> )	6		XPS	01D1
		Ni(3p <sub>3/2</sub> )	853.7 - 553.9, 855.5 - 855.9			
	c(2×2)O		-1 - -4	O(2p) hybridized with Ni(s,p), strong dispersion of up to 3 eV	IPE, KRIPES	94H1
	c(2×2)O		5.5	O(2p) derived state (hybrid of O(2p) and Ni-4s4p)	theory	85G2, 71E1
	c(2×2)O	O(1s)	529.9		UPS	89N1
	c(2×2)O		524	O-K emission	SCLS	92W2
	(2×2)O	O(1s)	529.75		SXES	89N1
	(2×2)O	O(2p <sub>z</sub> )	8		SCLS	89N1
		O(2p <sub>x,y</sub> )	6		UPS	64G1, 77J1
	30 L O <sub>2</sub> , 100 K	O(1s)	530		XPS	95R2, 00K1
			531.5			
	(2×2)O			Oxygen K-emission spectra: 2p-3d anti-bonding state partly occupied.	SXES	93T1
Pd(110)	c(2×4)O	Pd(3d <sub>5/2</sub> )	335.58 336.3	clean surface component 334.96 eV	SCLS	91C1
			6	surface oxide	SCLS	96B1
	c(2×4)O	O(2p <sub>z</sub> )		1 eV dispersion along densely packed rows.	ARUPS	93Y1
Pd(111)	100 L O <sub>2</sub> , 300 K	O(2s)	21.2, 22.2	O chemisorbed	UPS	83W1
	100 L O <sub>2</sub> , 1000 K	O(2s)	24.3	O subsurface		
	0.4 ML	Pd(3d <sub>5/2</sub> )	335.0		XPS	90B1
		O(1s)	532.3			
	>3 ML	Pd(3d <sub>5/2</sub> )	336.6			
Pd(100)	c(2×2)	O(1s)	529.6		PES	94G1, 96P1
		Pd(3d <sub>5/2</sub> )	335.54	clean surface 335.40 eV; angular dependence of the intensity: O in 4-fold hollow 0.92 Å above the Pd layer.		
Pt(110)	(1×2)MR+O <sub>2</sub>	O(1s)	529.9		XPS	86F1
	(1×2)MS+O <sub>2</sub>	O(1s)	529.9			
Pt(111)	(2×2)O	O(2p)	6.5			89P1, 80G1

Substrate	Surface	State	Binding energy [eV]	Remarks	Method	Ref.
Pt(111) cont.	0.2 - 0.8 ML	O(1s)	530.8	strong interaction between O(2p) and Pt-5d	XPS	84D1
		O(1s)	529.8			80G2
Pt(100)- (1×1)		O(2p)	6		UPS	76H2, 84N2
	0.2 ML	O(1s)	530.9		theory	92B1
	0.8 ML	O(1s)	529.8		XPS	84D1
Re(0001)	-	O(1s)	530		XPS	80D3
		O(2p)	6		UPS	
Re(10 $\bar{1}$ 0)	(1×5)2O			O(2p <sub>x</sub> ) and O(2p <sub>z</sub> ) disperse by about 1.0 eV along the close-packed Re rows. No dispersion perpendicular to the Re rows.	ARUPS	92L2
	(1×3)2O					
	c(2×4)O	O(2p)	5.5, 6.6, 7.8	3 weakly dispersing O(2p) bands	ARUPS	92L3
Rh(110)	disordered			low temperature adsorption		94C1
	<0.3 ML	O(1s)	529.65	2 O-induced states (2p <sub>z</sub> , 2p <sub>x</sub> ) disperse by 1.2 eV and 0.8 eV	ARUPS	98C1
	>0.8 ML	O(1s)	530.25			
	(2×2)p2mg				CLS	01V1
	(2×2)p2mg (10×2)	O(1s) O(1s)	530.25 529.75			
Rh(111)	(2×2)O	O(1s)	529.4	Rh c.t 1O w.r.t. bulk Rh c.t 2O w.r.t. bulk	PES	99J1
	(2×1)O	O(1s)	529.4		SCLS	00A2
	(2×2)O	Rh(3d <sub>5/2</sub> )	-0.12			
	(2×1)O	Rh(3d <sub>5/2</sub> )	0.3			
Rh(100)	(2×2)4pg	O(2p <sub>z</sub> )	5.9	derived states disperse by about 1.4 eV	PES	96Z1
		O(2s)	21.0	w.r.t. bulk	SCLS	
		Rh(3d <sub>5/2</sub> )	-0.25			
	(2×2)4pg	O(1s)	529.8±0.2		XPS	83F2
Ru(10 $\bar{1}$ 0)	c(2×4)2O		4.0, 4.7, 5.2, 5.8, 6.2, 6.8	6 O-induced bands; all of them are weakly dispersing (<0.1 eV)		93R1
	c(2×4)2O, (2×1)p2mg-2O	Ru(3d <sub>5/2</sub> )	0.395 (Ru-O) 0.695 (Ru-2O)	shift by 75 meV 5 O(2p) induced bands for various polarizations of the light	SCLS	00B1
	(2×1)p2mg-2O	O(1s)	2.8, 4.2, 4.6, 5.0, 6.3			
						95R1
Ru(0001)	<0.50 ML	O(1s)	529.8±0.2			75F1
		O(2p) induced states	6.4			
	≤1.0 ML	O(1s)	530.24			01O1

Substrate	Surface	State	Binding energy [eV]	Remarks	Method	Ref.
Ru(0001) cont.	(2×2)O		280.1	surface		00L1
	(2×1)O		280.60	surface		01O1, 00L1
	(2×2)3O		281.04, 280.66	surface		01O1, 00L1
	(1×1)O		281.04	surface		01O1
Ta(110)	0.5 L O <sub>2</sub>	Ta(4f <sub>7/2</sub> )	23	clean	PES	95R3
			24.1	(2×1)O		
			24.9	coplanar Ta+O layer		
			27.5	Ta <sub>2</sub> O <sub>5</sub>		
Ta(111)	1 L O <sub>2</sub>	Ta(4f <sub>7/2</sub> )	22.76		PES	82V1
	5 L O <sub>2</sub>	Ta(4f <sub>7/2</sub> )	22.94, 24.04, 22.14			
Ti(0001)				Surface state of Ti(0001) just above $E_F$ disappears upon O-exposure.	APS	81J1
			O(2p)	5.9	UPS	81H2
V(110)	c(2×6)	V(2p <sub>1/2</sub> ), V(2p <sub>3/2</sub> ), O(1s)	only kinetic energies are given			00G2
V(111)	<10 L O <sub>2</sub>	V(2p <sub>1/2</sub> )	524		XPS, UPS	91S3
		V(2p <sub>3/2</sub> )	516			
		O(1s)	534			
		O(2p)	5 - 6			
V(100)	(1×5)O	V(2p <sub>1/2</sub> )	519.7		XPS	10S1, 83F4
		V(2p <sub>3/2</sub> )	512.2			
		O(1s)	531			
		O(2p)	5 - 7	O segregation		
W(110)	(2×1)-O	W(4f <sub>7/2</sub> )	31.7		SCLS	94P1, 98R1
	(1×1)-1O	W(4f <sub>7/2</sub> )	32.0		XPS	98D1, 98D2,
		clean W(4f <sub>7/2</sub> )	31.1		SCL	98R1
	(1×1)-1O	W(4f <sub>7/2</sub> )		shift 0.60 eV	FLAPW	99O1
	0.50 - 1.0 ML	O(2p)	6.3		UPS, 100 eV	94P1
	(1×1)O	O(2p)	5.1, 6.1, 7.7		PES	99F1
		O(1s)	530.35		XPS	81O1
W(111)	0.1 L O <sub>2</sub>	W(4f <sub>7/2</sub> )	31.83		PES	82V1
	0.7 L O <sub>2</sub>	W(4f <sub>7/2</sub> )	31.73			
	initial	O(1s)	530.35		XPS	74Y1
W(100)	(1×1), <0.5 ML	W(4f <sub>7/2</sub> )	31.13 → 31.9		SCLS	89A1
	(1×1) 1 ML	W(4f <sub>7/2</sub> )	31.13 → 33.2			
	(2×1)	W(4f <sub>7/2</sub> )	31.13 → 32.8			
	(4×1)	O(2p)	-2.3	WO <sub>2</sub> like phase reconstructed 2D "WO <sub>2</sub> "	KRIPES	88K2

Substrate	Surface	State	Binding energy [eV]	Remarks	Method	Ref.
Zn(0001)	100 L cluster 1 - 1000 L	O(2p)	4.3 - 5	strong bonding character	UPS	75B1, 78A1
		O(2p) and Zn(4s, 4p)			DV-X $\alpha$ -MO	83M3
		O(1s)	530		XPS	85S4
Zr(0001)	(1 $\times$ 1)O		6, 7.6	O-derived bands	theory	96Y1
	(2 $\times$ 1)O					

### 3.4.2.2.5 Vibrational properties of chemisorbed oxygen

**Table 5.** Vibrational properties of (atomic) oxygen overlayers on metal surfaces and the beginning of surface oxide formation. Suggested adsorption sites are indicated. If not otherwise indicated the technique of HREELS or IRAS was used.

substrate	structure	Me-O stretch vibration [meV]	adsorption site	Ref.
Ag(110)	(2×1)	39, 41 surface phonon: 17 anharmonicity		81B3, 80S1 95S1
	(2×1), (3×1), (4×1)	40.9, 40.2, 39.8		94S2
	low cov.	38.5		94S2
	O(β)	78.5	subsurface	94P3/SERS
	O(γ)	104	on-surface	94P3/SERS
	c(6×2)O	37.2, 42.4		95B5
Ag(111)	disordered O	30	-	83B3, 95B3
	O(β)	78.5	dissolved O	94P3/SERS
	O(β)	80.8		95B7/Raman
	O(γ)	104	embedded O	94P3/SERS
	O(γ)	104		95B7/Raman
Ag(100)	c(2×2)	37	fourfold hollow	90A1
	(1×1)	30		
Al(111)	isolated O	50 - 54	fcc hollow	86C1
	(1×1)O	65 - 81	on- and subsurface-O; O-islands	87A1
	(1×1)O	65 - 81	subsurface-O	87A1
	(1×1)O	105	oxidic O	82E3
		105 - 120	fcc-hollow	87A1
	(1×1)O islands	re-interpretation: 72, 60, 105 Motion of the Al <sub>3</sub> O coordination cluster: perpendicular, umbrella, lateral.		96F1, 97H1
Co(10 $\bar{1}$ 0)	c(2×4), p(2×1)	50 - 65	C <sub>1</sub> symmetry	90S1
	(2×1)pg-2O		C <sub>s</sub> symmetry	90S1
			no C <sub>2v</sub> symm.	
Cr(110)	initial	76.9	long-bridge	86S3, 86S4
	p(4×2)	75.6	long-bridge	86S3, 86S4
Cr(100)	0.75L O <sub>2</sub> at RT	68	-	86B4
	5L O <sub>2</sub> at RT	65	-	86B4
Cr(111)	0.6 - 1.5 L O <sub>2</sub> at RT	44, 72.5	-	86B5
Cu(110)	(2×1)	29.6, parallel [1 $\bar{1}$ 0]	long-bridge	90V1
		48.5, perpendicular [1 $\bar{1}$ 0]		87M1
	c(6×2)	48.5	long-bridge	87M1
		42.1, 62	O-3Cu	
Cu(111)	disordered	29.4	threefold hollow	82D1

substrate	structure	Me-O stretch vibration [meV]	adsorption site	Ref.
Cu(100)	(2√2×√2)R45°	36, 55.2, 84.9	fourfold hollow	89W1
Fe(110)	p(2×2)	62.5	long-bridge	81E1
	c(3×1)	69	long-bridge	81E1
Fe(100)	p(1×1)O	54, 35	4-fold	90L2
	LT phase	56, 81	4,1-fold	89L2
Fe(111)		62 - 66 coverage dependent	-	86B2
Ir(111)	0 - 0.52 ML subs. O	68	threefold	87M1
		100		87M1
Mg(0001) Mg(10 $\bar{1}$ 0)	<10 L O <sub>2</sub>	57, 77	MgO FK , interstitial O	89T1
Mo(110)	p(2×2)O LT >0.25 ML LT 1000 K dose	66 (adsorbed O)	long-bridge	92C2, 98K4
		47, 75 (adsorbed O)	3-fold	92C2
		92.5 (oxide layer)		92C2
Mo(111)	0.8 ML	51, 77	threefold	88S1
		121.6	on-top	88S1
Mo(100)	(√5×√5)R26°	70	3-fold	83M2
	(√5×√5)R26°	55, 69, (91)	3-fold (on-top)	00K1
	(2×1)	62, 74, 94	MoO <sub>2</sub>	00K1
	(1×1)O	67.5, 51, 67, 82	oxidized surface	83M2
Ni(110)	(2×1)	24, 46	long-bridge	90V1
Ni(111)	(2×2)	72	threefold hollow	80I1
	(√3×√3)R30°	72	-	80I1
	(2×2)O	surface phonon		94T1
Ni(100)	p(2×2)	53	fourfold hollow	83A1, 84R1
	c(2×2)	39		83A1, 84R1
	disordered	49 (0.11 ML), 46 (0.56 ML)		85R1
	c(2×2)	77, 88, 98, 105, 121	5 types of subsurface oxygen	93O1
Ni(113)	0 - 0.5ML	55 - 65, 149 - 155	3-fold	96S6
		35 - 40, 85 - 90	4-fold	96S6
		100, 124	O between rows	96S6
Pd(110)	(2×3)-1D	32, 59	long-bridge	87K1, 86N1
	c(2×4),	56	long-bridge	86N1
	(2×3)-1D	56		86N1
Pd(111)	(2×2)O	59.4	3-fold hollow	86I1, 90B1
	(2×2)O	O-induced Raleigh-Ph.-gap		96K1
	>1.4 ML	34, 53, 84, 94	surface oxide	90B1
Pd(100)	(2×2)-O	44	4-fold hollow	91S1, 82N1, 84S1
	c(2×2)-O	44	4-fold hollow	91S1, 82N1 84S1
	p(5×5)	44, 50	reconstruction	91S1
	(√5×√5)	44, 54	reconstruction	91S1
Pt(110)- 2×1		60, 41 perpendicular and lateral Pt-O vibration	fcc site	93S1

substrate	structure	Me-O stretch vibration [meV]	adsorption site	Ref.
Pt(111)	(2×2)1O	58 (perp. vibration)	3-fold hollow	89P1, 82S3
	(2×2)3O	59.4	3-fold hollow	89P1
Pt(322)	“oxide”	95	“oxide”	80G1
	low cov.	70	O adsorbed in edge bridge of A-type steps	97W2, 98F1
Rh(110)	low cov.	72	long-bridge	93A1
	(2×1)p2mg	45, 63		
	(2×2)p2mg	47, 65		
Rh(111)	(2×2), (2×1)	62 - 68	threefold hollow	86R1
Rh(100)	(2×2)	48 - 54	fourfold hollow	82S1, 90F1, 87G1, 82D3
	c(2×2)			
	(2×2)4p4g			
Ru(10 $\bar{1}$ 0)	c(2×4)-2O	67	3-fold	98S1
	(2×1)pg-2O	64	3-fold	98S1
Ru(0001)	initial	54	3-fold	97H1
	(2×2)O	64	3-fold	79T3, 95M1
	(2×1)O	73 (perp.), 53 (lateral)	3-fold	79T3, 97K1
	(2×2)3O	80 (perp.), 67 (lateral)	3-fold	97K1
	(1×1)O	81 (perp.)	3-fold	97H1
V(110)		77	on-surface	95K2
		131	sub-surface	95K2
W(110)	initial	69.5	long-bridge	84D1
	(2×1)O	72, 48	quasi-3-fold	84D1, 97E1
	(2×2)3O	79, 50	quasi-3-fold	97E1
	(1×1)O	82, 53	quasi-3-fold	97E1
W(100)	0.17 ML	75	3-fold	76F1
	0.27 ML	50, 78		76F1
	0.45 ML	50, 78, 90		76F1
	1.0 ML	65, 90	oxide	76F1
		127.5	on-top	76F1
Ti(0001)	(2×2)O	65	octahedral	90G1, 85S1
	25 L	65, 87		90G1
	(1×1)O	40 - 45, 90 - 92		85 S1
Zn(0001)	1 - 30 L O <sub>2</sub>	70.5	oxide layer	85S4
	100-1000 L O <sub>2</sub>	70.5, 49		
Zr(0001)	(1×1)O	60 (theory)	octahedral	96Y1

### 3.4.2.2.6 Local atomic oxygen-metal geometry

**Table 6.** The O-metal bond length and other structural characteristics.

substrate	surface	O-metal [ $\text{\AA}$ ]	Adsorption site/Remarks	Ref./Method
Ag(110)	(2 $\times$ 1)-O	2.04	MR reconstruction O in long-bridge	84P1/SEXAFS 93C2/ICISS
	(2 $\times$ 1)-O	2.13	MR, O in long-bridge	93S1/DFT
	c(6 $\times$ 2)-4O	2.05, 2.07	MR reconstruction analog to Cu(110)-c(6 $\times$ 2)	93D1/LEIS
	(1 $\times$ 2)-1O	-	every 2nd row missing	98O3/STM
Ag(111)	1 bar, 400 h, 800 K		subsurface induced reconstruction.	93B6/STM, RHEED, REM
	(4 $\times$ 4)-4O		Trilayer of Ag <sub>2</sub> O(111) on Ag(111) rotated by 30°	74R1/LEED
	(4 $\times$ 4)-4O		Ag-deficient trilayer	00C1/STM&DFT
Al(111)	(1 $\times$ 1)O	1.8	fcc, (1 $\times$ 1)O islands	92K1, 95J1, 01K2/DFT
	(1 $\times$ 1)O	1.92	fcc assumed	81B1/SEXAFS
	(1 $\times$ 1)O	1.76	3-fold coordinated.	81N2/SEXAFS
	(1 $\times$ 1)O	1.80	O fcc	81S1, 82N2, 83M1/ LEED
	(1 $\times$ 1)O	1.80	O fcc O-Al distance: 0.58 $\text{\AA}$	92K1/SXW
	(1 $\times$ 1)O	-	subsurface O ruled out	93W1/MEIS
	(1 $\times$ 1)O	-	O(1 $\times$ 1) islands + oxide	98M1/NDRS
	>0.1 ML	-	O-O distance 2.90 $\pm$ 0.05 $\text{\AA}$	93B2, 98T1/STM
	chemisorbed O	1.79 $\pm$ 0.05		80S3/SEXAFS
	oxidic O	1.88 $\pm$ 0.03		80S3/SEXAFS
Al(100)	(1 $\times$ 1)O	1.79		81W1/SC-LAPW
	low O cov.	2.14	4-fold	86M1/cluster calc.
	low O cov	1.75	4-fold	98D3/cluster calc.
	<0.30 ML	-	4-fold, O almost within the Al surface plane, randomly.	90L1, 91L2/ ARSIMS
	>0.30 ML		oxide phase starts to grow	80D2/LEED
	(1 $\times$ 1)O	1.98	4-fold	91L2/ARSIMS 80D2/EXAFS
Au(111)	( $\sqrt{3}\times\sqrt{3}$ )R30°	-	“gold oxide”	96H1/STM
Co(10 $\bar{1}$ 0)	(2 $\times$ 1)pg	1.83/1.99	O hcp like sites	97G2/LEED
fcc- Co(100)	c(2 $\times$ 2)O	1.94	O 4-fold hollow	78M3/LEED
Cr(100)	( $\sqrt{5}\times\sqrt{5}$ )R26°-5O	2.05	Cr vacancy structure	99S1/LEED-STM



substrate	surface	O-metal [ $\text{\AA}$ ]	Adsorption site/Remarks	Ref./Method
Cu(110)	(2 $\times$ 1)-O	1.84	O: long bridge, MR reconstruction	86B1/SEXAFS
		1.81, 2.00		91D1/ICISS
		1.84, 1.85		90F2/SXRD
		1.81, 2.01		90P2/LEED
		1.81, 1.77		93D1/LEIS
		1.89, 2.27		93S4/DFT
		1.83, 2.09		98F2/DFT
		1.83, 2.08		98L2/DFT
		-	MR, O: long-bridge; super Cu atom links two Cu/O chains; In-plane structure only.	90F3/SXRD
	c(6 $\times$ 2)-4O	1.78, 1.89 1.90	averaged Cu-O bond length	93D2/ICISS 95L1/LEED
Cu(111)	$\sqrt{73}R5.8^\circ \times \sqrt{21}R10.9^\circ$ single O	- 1.93	Added CuO <sub>2</sub> oxide layer 3-fold hollow assumed	01M1/STM 01G1/cluster
	(2 $\sqrt{2} \times \sqrt{2}$ )R45 $^\circ$ disordered	1.82, 2.14 1.86, 2.07 1.88, 2.07	O: 4-fold, MR reconstruction O: 4-fold, MR reconstruction O: 4-fold, unreconstructed	90Z1/LEED 93L1/SEXAFS 93L1/SEXAFS
Fe(110)	c(2 $\times$ 2)O	-	O-overlayer, O: long-bridge	95W1/STM
	c(3 $\times$ 1)	-	MR reconstruction	95W1/STM
	>0.4 ML	-	FeO islands grow	95W1/STM
Fe(211)	(2 $\times$ 1)O	2.05, 1.95	O: long-bridge, MR reconstruction	86S1/LEED
Fe(100)	(1 $\times$ 1)O	2.07, 2.00	O: deep in 4-fold hollow sites	77L2, 87J1/LEED
	(1 $\times$ 1)O	2.02		81R1/Theory
	(1 $\times$ 1)O	2.10		87V1/LEIS
	(1 $\times$ 1)O	2.06, 1.97		89H3/MEIS
	(1 $\times$ 1)O	2.06	Fe-Fe layer distance: +23 %	87C3/FLAPW
Ir(110)	c(2 $\times$ 2)-O	1.93 1.80	O: short bridge	78C2/LEED 95B6/TOF-SARS
Ir(111)	(2 $\times$ 2)-O	2.04	O: fcc	79C1/LEED
Ir(100)	(1 $\times$ 2)-O	1.95 1.93	O: bridge site O: bridge site	00J1/DFT 00J1/LEED
Mg(0001)	8 L O <sub>2</sub>	-	90 % on-surface, 10 % subsurface, Mg-O layer distance: 0.7 $\text{\AA}$ ; note the work function decreased by 1 eV.	98M2/NDRS
		2.70	O octahedral	89C1/FFAK
	(1 $\times$ 1)O	1.97, 2.08	O-tetrahedral, islanding	97B2/DFT
Mo(100)	( $\sqrt{5} \times \sqrt{5}$ )-4O	2.12, 1.6	4Mo+4O per unit cell with Mo-Mo bond length: 2.85 $\text{\AA}$	96X1/STM 92R1/SXRD
	(2 $\times$ 1)-2O	-	MR reconstruction	96X1/STM
	low O-cov.	-	O 4-fold without reconstruction	82O1/LEIS
Ni(110)	(2 $\times$ 1)O	1.78	O: long-bridge, MR	85N1/ICISS
	(2 $\times$ 1)O	1.77, 1.86	O: long-bridge, MR	90K1/LEED
	(1 $\times$ 2)O initially	-	every 2nd Ni row is missing	94E1/STM

substrate	surface	O-metal [ $\text{\AA}$ ]	Adsorption site/Remarks	Ref./Method
Ni(111)	(2 $\times$ 2)O	1.83	fcc	90V1, 94S1/LEED
	(2 $\times$ 2)O	1.85 $\pm$ 0.03	fcc	92H1/SEXAFS
	(2 $\times$ 2)O	1.85 $\pm$ 0.05	fcc	90P1/NEXAFS
	(2 $\times$ 2)O	1.80 $\pm$ 0.04	fcc	96D1/PhD
	( $\sqrt{3}\times\sqrt{3}$ )O	1.80 $\pm$ 0.02	fcc	91M1/LEED
	( $\sqrt{3}\times\sqrt{3}$ )O	1.85	fcc	92H1/SEXAFS
	( $\sqrt{3}\times\sqrt{3}$ )	1.87	fcc	81N3/HEIS
	0.3 ML	-	fcc, hcp (domain boundary)	96S5, 97S5/ DLEED
	>0.7 ML	-	oxide formation	01D1/XPS
Ni(100)	disord., <0.1 ML	1.94 $\pm$ 0.03	4-fold	91O1/LEED
	(2 $\times$ 2)O	1.93 $\pm$ 0.03	4-fold	91O1/LEED
	c(2 $\times$ 2)O	1.92 $\pm$ 0.03	4-fold	91O1/LEED
	c(2 $\times$ 2)O	1.96 $\pm$ 0.03	4-fold	82S2/SEXAFS
	p(2 $\times$ 2), c(2 $\times$ 2)	-	4-fold, $d(\text{O-Ni})=0.9 \text{ \AA}$	83N1/NEXAFS
	oxide form.	-	>80L visible in NEXAFS	83N1/NEXAFS
	c(2 $\times$ 2)O	1.92	4-fold	93S2/PhD
	c(2 $\times$ 2)O	1.92	4-fold	99A1/DFT
	p(2 $\times$ 2)O, c(2 $\times$ 2)O	1.96 $\pm$ 0.05	4-fold	94X1/SIMS
	(2 $\times$ 2)O	1.95 $\pm$ 0.05	4-fold	83F3/RBS
	(2 $\times$ 2)O	1.96 $\pm$ 0.05	4-fold	94X1/SIMS
	single O	1.93	4-fold	93G2/cluster theo.
Pd(110)	(2 $\times$ 3)	2.07, 1.80	fcc, (1 $\times$ 3) MR	89H2/RBS
	c(2 $\times$ 4)O	1.86, 1.88	fcc, (1 $\times$ 2) MR	97B1/LEED
	(2 $\times$ 2)mgO	2.02	fcc, (1 $\times$ 2) MR	97B1/LEED
	c(2 $\times$ 4), (2 $\times$ 3)-1D	-	reconstructed surface	01H1/DFT 98L1/DFT
Pd(111)	( $\sqrt{3}\times\sqrt{3}$ )O	2.03	fcc (assumed)	98O1/LEED
	(2 $\times$ 2)O	1.98 $\pm$ 0.08	fcc	98O1/LEED
	( $\sqrt{3}\times\sqrt{3}$ )O	2.02 $\pm$ 0.08	fcc	
Pd(100)	c(2 $\times$ 2)O	2.18	4-fold	98L1/DFT
	p(2 $\times$ 2)O	2.11	4-fold	96K2/LEED
	( $\sqrt{5}\times\sqrt{5}$ )R27 $^\circ$ O	1.73	single PdO(001) on Pd(100)	94V3/LEED
Pt(210)	(5 $\times$ 2)rect-O	1.79 $\pm$ 0.05	3-fold on both (110) and (310) facets	94L1/SEXAFS
Pt(100)	c(2 $\times$ 2)-1O	1.94	O: bridge	97G1/DFT
	p(2 $\times$ 2)-1O	1.94	O: bridge and 4-fold site are energetically degenerated	97G1/DFT
Rh(110)	(2 $\times$ 2)p2mg-2O	2.0 $\pm$ 0.1	fcc, (1 $\times$ 2) MR	93G1/LEED
	c(2 $\times$ 8)-12O	-	fcc, (1 $\times$ 4) MR	94O1/LEED
	(5 $\times$ 10)np	-	fcc	95O1/LEED
	(2 $\times$ 1)pmg-2O	1.97, 2.02	fcc	93G1, 95B1/LEED
	(2 $\times$ 2)	2.00	(1 $\times$ 2)MR, O fcc	97S5/DFT

substrate	surface	O-metal [ $\text{\AA}$ ]	Adsorption site/Remarks	Ref./Method
Rh(111)	$(\sqrt{3}\times\sqrt{3})\text{O}$	2.0	fcc (assumed)	98L1/DFT
	$(2\times 2)\text{O}$	$2.00\pm 0.08$	fcc	97S3, 86W1/LEED
	$(2\times 1)\text{O}$	$2.02\pm 0.08$	fcc	97S3, 96W1/LEED
	$(2\times 2)\text{O}$	2.00	fcc	99G1/DFT
	$(2\times 1)\text{O}$	1.99	fcc	99G1/DFT
	$(1\times 1)\text{O}$	1.95	fcc	99G1/DFT
	O subsurface	1.8	octahedral	98W1/PhD
	Single O	2.02	fcc, assumed	97C3/cluster
Rh(100)	$c(2\times 2)\text{O}$	2.17	4-fold	98L1/ DFT
	$(2\times 2)\text{O}$	$2.12\pm 0.06$	4-fold	88O1/ LEED
	$(2\times 2)4\text{pg-}2\text{O}$	2.00, 2.06	quasi-3-fold, clock reconstruction type 2 <sup>a</sup> ), 0.2 $\text{\AA}$ displacements of Rh atoms	99A1/DFT 98S7, 99B1/LEED 99N1/SXRD
Ru( $10\bar{1}0$ )	$c(2\times 4)\text{-}2\text{O}$	2.08, 2.03	hcp along the Ru flanks	98S1/LEED
	$(2\times 1)\text{p}2\text{mg-}2\text{O}$	2.03, 2.03	hcp along the Ru flanks	98S1/LEED
	$c(2\times 4)\text{-}2\text{O}$	2.09, 2.10	hcp	98S1/DFT
	$(2\times 1)\text{p}2\text{mg-}2\text{O}$	2.11, 2.11	hcp	98S1/DFT
	$(1\times 1)2\text{O}$	1.98, 2.08	fcc, hcp	98S1/DFT
	artificial			
Ru(0001)	$(2\times 2)\text{O}$	$2.03\pm 0.06$	hcp	89L1/LEED
	$(2\times 1)\text{O}$	$2.02\pm 0.06$	hcp	89P1/LEED
	$(2\times 2)3\text{O}$	$11.98\pm 0.0$	hcp	98K2/LEED
	$(1\times 1)\text{O}$	6	hcp	96S3/LEED
	$(2\times 2)\text{O}$	$2.00\pm 0.04$	hcp	96S2/DFT
	$(2\times 1)\text{O}$	22.10	hcp	96S2/DFT
	$(1\times 1)\text{O}$	2.08	hcp	96S2/DFT
	stepped Ru(0001)	2.03	hcp (terrace), four-fold (step)	95H1/LEED
		-		
Ta(100)	$(3\times 1)\text{-O}$	$2.0\pm 0.1$	4-fold interstitial	85T1/LEED
W(110)	$(2\times 1)\text{O}$	2.08	3-fold	75V1/LEED
	$(2\times 1)\text{O}$	2.05, 2.11	3-fold	01Y1/LEED
	$(2\times 1)\text{O}$		3-fold	93J1/STM
	$\approx(1\times 1)\text{O}$	1.73	3-fold	98D1, 01T1/PhD
	$(1\times 1)\text{O}$		two types of 3-fold O	93J1/STM
	$(1\times 1)\text{O}$	-	W-O layer distance: 1.18 $\text{\AA}$	99O1/XPD
W(100)	O disordered	2.10	4-fold	86R1/DLEED
W(100)	$(4\times 1)$	1.65	-----	98O2/EELFS
W(211)	$(2\times 1)\text{-}3\text{O}$	2.0, 2.24	3-fold trough	89B1, 89R2/TOF-SARS
W(100)- 2 $\times$ 1	O disordered	-	O disordered in 2nd layer, MR 3-fold or 4-fold hollow, MR	89M1/LEIS 91M2/STM

substrate	surface	O-metal [ $\text{\AA}$ ]	Adsorption site/Remarks	Ref./Method
Zr(0001)	(2 $\times$ 2)2O	2.28 $\pm$ 0.05	O-octahedral below 1st and 2nd layer	95W1/LEED
	(2 $\times$ 1)O	2.11	O-octahedral below 1st and 2nd layer	01J1/DFT
	(1 $\times$ 1)1O	2.28	0.5 ML below 1st and 0.5 ML below 2nd layer (octahedral)	95W2/LEED
	(1 $\times$ 1)1O	2.05	O-octahedral	01J1/DFT
	(1 $\times$ 1)2O	2.21, 2.07	tetrahedral/on-surface similar to ZrO <sub>2</sub>	97W1/LEED

Remarks:

- a) Clock reconstruction type 1 (black) and type 2 (white) according to 99A1  
b) In general, DFT slab calculations are more reliable than Cluster calculations concerning the atomic geometries.

### 3.4.2.2.7 Ordered overlayers of chemisorbed oxygen and surface oxides on metal surfaces

**Table 7.** Ordered overlayers of chemisorbed oxygen and surface oxides on metal surfaces.

Substrate	Orientation	O-surface structure	Ref.
fcc-Ag	(110)	(2 $\times$ 1), (3 $\times$ 1), (4 $\times$ 1), (5 $\times$ 1), (6 $\times$ 1), (7 $\times$ 1), c(6 $\times$ 2)-6O	73E1, 76E1, 84C1
	(110)	c(2 $\times$ 2) high pressure phase	88S2
	(331)	(2 $\times$ 1)	78M1
	(111)	(2 $\times$ 2), ( $\sqrt{3}\times\sqrt{3}$ )R30°, (4 $\times$ 4)-4O	65M1, 74R1 85C1, 95B5
	(100)	disordered, c(2 $\times$ 2)	76E1, 85G1
fcc-Al	(110)	(331) facets, (111) facets	71B1, 72V1
	(111)	(4 $\times$ 4), (1 $\times$ 1)O, oxide-like (1 $\times$ 1)O islands	71B1, 78F1, 83M1, 93B2, 98T1 88W2/STM
	(100)	disordered, amorphous oxide	67J1, 77F1
fcc-Au	(111)	( $\sqrt{3}\times\sqrt{3}$ )R30°	96C1
hcp-Be	(0001)	(1 $\times$ 1)O, BeO(0001)-(1 $\times$ 1), BeO(0001)-(2 $\times$ 2)	84F1
hcp-Co	(10 $\bar{1}$ 0)	(2 $\times$ 1), c(2 $\times$ 4), (2 $\times$ 1)pg	90S1
	(0001)	disordered	82C1
fcc-Co	(100)	(2 $\times$ 2), c(2 $\times$ 2) and then nucleation of CoO crystallites.	77R1
bcc-Cr	(110)	(3 $\times$ 1), (100)-facets p(4 $\times$ 2)	73M1 88K3
	(111)	( $\sqrt{3}\times\sqrt{3}$ )R30°	78J1
	(100)	c(2 $\times$ 2), c(2 $\times$ 4), (1 $\times$ 1)	77H1, 82G1
fcc-Cu	(110)	(2 $\times$ 1), c(6 $\times$ 2)	67E1, 83F1
	(210)	(2 $\times$ 1), (3 $\times$ 1)	78M2
	(111)	disordered, (4,3,-3,5)	67E1
	(332)	disordered, (9,1,1,5)	82M1
	(100)	(2 $\sqrt{2}\times\sqrt{2}$ )R45°, c(2 $\times$ 2)	79W1, 98T2
	(h11)	c(2 $\times$ 2)	92S1
	h=5,...,15		

Substrate	Orientation	O-surface structure	Ref.
bcc-Fe	(110)	c(2×2), (3×1), (2×2) beyond 0.4ML O: FeO(111)	62G1, 84K1 95W4
	(111)	(6×6), (5×5), (4×4), (2√7×2√7)R19.1°, (2√3×2√3)R30°	77N1
	(100)	c(2×2), (1×1)O	76B1
hcp-Gd	(0001)	(1×1)-disordered	86W3, 95Z1
fcc-Ir	(110)	(2×2), c(2×2), (3×2), (1×1), (1×4)- oxide	79T1
	(111)	(2×2) or/and (2×1)	71G1, 79C1
	(766)	(2×1)	76H1
	(100)	(2×1), (5×1), (1×1)	69G1, 76R1, 81H1
hcp-Mg	(0001)	(1×1) disordered, MgO(111)(1×1)R30°, MgO(111)(√7×√7/2)R19°	81N1, 82F1
bcc-Mo	(110)	(2×2)-1O, (2×1)-O, (1×1) 1-dim. ordered structures	68H1, 89G2, 91D2, 86W2, 89G2 96K1/RHEED
	(111)	(211) facets, (110) facets, (4×2), (4×4), (1×3), (112)-(1×2) facets, (112)-(1×3) facets	77C1, 75K1, 85Z1
	(211)	(2×1), (1×2), (1×3), c(4×2)	70D1
	(100)	c(4×4), (2×1), (√5×√5)R26°, (4×1) c(2×2), (6×2), (3×1), (5×5), (110) and (112)facets	68H1, 69K1, 77C1, 75R1, 85Z1, 79B2
		(1×1)O	83M2
bcc-Nb	(110)	(3×1)	67H1
	(111)	(2×2), (1×1)	77P1
	(100)	c(2×2), (1×1), (3×10)-oxide	77P1, 73F1
fcc-Ni	(110)	c(2×4), (2×1), (3×1), (9×4)	85B1, 64M1, 68M1, 93B1
	(771)	(2×1)	91H1
	(111)	(2×2), (√3×√3)R30°	64M1, 81K1
	(100)	(2×2), c(2×2)	64M1, 83D1
fcc-Pd	(110)	(1×3), (1×2), pseudo-(2×1), c(2×6), c(2×4)-4O	69E1, 89H2
	(331)	(1,2,2,0)	81D1
	(111)	(2×2), (√3×√3)R30°, (2×2)-oxide	77C2
	(100)	(2×2), c(2×2), (√5×√5), (5×5)	82O1, 87C1, 88C1, 91S1
fcc-Pt	(110)	(2×1), (4×2), c(2×2), (1×3), (1×5), (1×7)	64T1, 76D1, 80S1
	(111)	(2×2)-O, (√3×√3)R30°, (4√3×4√3)R30°, PtO <sub>2</sub> (0001), (3×15)	64T2, 77W1, 77L1
		(2×2)-3O	89P2
	(654)	(√3×√3)R30°	80D1
	(766)	(2×2), (√3×√3)R30°	77L1
	(12,9,8)	(√3×√3)R30°	80D1
	(62,62,60)	(2×2)	80D1

Substrate	Orientation	O-surface structure	Ref.
fcc-Pt (cont.)	(100)	( $2\sqrt{2}\times 2\sqrt{2}$ )R45°, (5×1), ( $2\sqrt{2}\times\sqrt{2}$ )R45°, (2×1), (3×1)	77L1, 79M1, 77P2, 84B1
	(611)	( $2\sqrt{2}\times\sqrt{2}$ )R45°	79M1, 83L1
hcp-Re	(10 $\bar{1}$ 0)	(2×3)O, c(2×4)2O, (1×5)2O, (1×4)2O, (1×3)2O	91L1, 72Z1
	(0001)	(2×2)	69F1, 70D2
fcc-Rh	(110)	(2×2)p2mg-2O, (2×3)p2mg, c(2×2 <i>n</i> )3 <i>n</i> O, <i>n</i> =3,4,5, ... (2×1)p2mg-2O (10×2)	66T1, 67T1, 90S2, 91B1  01V1
	(331)	(2×1), (1×3)	93V1, 95F1
	(111)	(2×2), (2×1), (8×8)-oxide	79T2, 80C1
	(111)	(1×1)	99G1
	(755), (331)	(2×2)	79C1
	(100)	(2×2), (2×2)gg,	78C1, 88O1
	(10 $\bar{1}$ 0)	c(4×2), (2×1)p2mg, c(2×6), (7×1)	77O1
hcp-Ru	(101)	(1,1,3,0), (2,1,5,0), (4,1,9,0)	77R2
	(0001)	(2×2), (2×1), (2×2)-3O, (1×1)O (2×1)O	70G1, 75M1, 82D1, 97K1, 96S1 79P1
fcc-Ta	(110)	(3×1)	67H1
	(100)	(2×8/9), c(3×1), (4×1), (3×3), (1×2), (1×3)	74C1, 85T1
	(211)	(3×1)	67H1
hcp-Ti	(0001)	(1×1), (2×2)O	58F1, 81J1, 85S1, 90G1
fcc-Th	(111)	disordered	77B1
	(100)	disordered	76T1
bcc-V	(110)	(3×1), c(6×2)	67H1, 00G2
	(100)	(5×1)	82J3, 84G1
bcc-W	(110)	(2×1)-O, (2×2)-3O, (1×1)-1O, c(14×7), c(2×2), c(21×7), c(48×16)	75E1, 78C3, 93J1, 67T2 73B1, 66G1, 78B2
	(10,1,1)	(2×1)	77E1
	(111)	disordered, (211) facets	79N1
	(100)	disordered, (4×1), (2×2), (2×1), (3×3), c(2×2), c(8×2), (3×1), (8×1), (4×4)	73P1, 76B1, 81K2
	(211), (221)	(2×1), (1× <i>n</i> ), <i>n</i> = 1, 2, ..., 7	67C1, 83W2, 85B1, 85W2
	(10 $\bar{1}$ 0)	(2×4)	94Z1
hcp-Zr	(0001)	(2×2)2O, (1×1)1O, (1×1)2O	95W1, 95W2, 97W1
	(10 $\bar{1}$ 0)	(2×4)	94Z1

Remarks:

- a) (1×1) can mean ordered (1×1)O phase or disordered phase, while (1×1)O is used for an ordered (1×1) overlayer of oxygen.
- b) Disorder occurs more frequently on (100) presumably due to higher diffusion barriers.

### 3.4.2.2.8 Phase diagrams and phase transitions in the O-metal surface system

**Table 8.** Phase diagrams and phase transitions of O-metal systems.

substrate	surface	phase diagram/remarks/kind of order-disorder transition/critical temperature $T_c$	Ref./method
fcc-Ag	(100)	c(2×2)O → (1×1)O phase transition at 180 K < $T$ < 293 K	90A1/HREELS
Cu(110)	(2×1)O	Evolution of the (2×1)O added row reconstruction	90C2/STM
Mo(110)	(2×2)-(2×1)	order-order phase transitions with non-universal behavior	91D2/MCS 86W2/LEED
	(2×2)-(1×1)	order-disorder transition: XY model	90G2/LEED
Ni(110)	(2×1)O	Stepped (110): evolution of the (2×1)O	82K2/STM
	(3×1)O, (2×1)O	(3×1)O, (2×1)O, (3×1)2O	80S1/RBS
Ni(111)	(2×2)O	$T_c = 438$ K, 4-state Potts model	95L2
	(2×2)O	$T_c = 439.5$ K, neither Ising nor 4-state Potts, $\alpha = 0.80 \pm 0.04$	94S1
	( $\sqrt{3} \times \sqrt{3}$ )R30°-O phase diagram	3-state Potts model (2×2)O, ( $\sqrt{3} \times \sqrt{3}$ )R30°-O	87P1/LEED 81K1/LEED
Ni(100)	(2×2)O, c(2×2)	Transition from (2×2) to c(2×2)	85R1/HREELS 83R3/HeD
Pd(100)	(2×2)	$T_c = 550$ K	87C4/LEED
	c(2×2)	$T_c = 590$ K, $T$ - $\theta$ phase diagram	
Rh(110)	(2×2)pmg	(2×2)pmg-(2×1) transition: 2D Ising model, $T_c = 750$ K	93B8/HeD
	(1× $n$ )	Missing Row Reconstructions	97K2/MC
Rh(111)	(2×2)O	4-states Potts model; $T_c = 280 \pm 5$ K	97O1/HeD, LEED
Rh(100)	(2×2)p4g	transition to c(2×2): 2-state Ising model; $T_c = 450 \pm 5$ K.	96B4/SPALEED
Ru(0001)	(2×2)O	$T_c = 754$ K, 4-state Pott	87P1/LEED
	(2×1)O	$T_c = 555$ K, 3-state Pott	90P3/LEED
W(110)	(2×1)O	$T_c = 709$ K, 2-D Ising model	93B8, 89W2/LEED
	(2×2)3O	3-particle interaction: 15 - 40 meV	78C3/MCS
	(2×2)3O	order-disorder: trans. may be 1st-order.	84R2
	(2×1)→(2×2)	universal class: XY model	82K1
	(2×1)+(2×2)	disordering kinetics	93J1
	(2×1)+(2×2)	phase separation	90T2/LEED
W(100)	(2×1)O→(1×1)	Deconstruction (order-order) phase transition, $T_c = 903$ K	92G1, 86R4/LEED
W(112)	(2×1)O	$T_c = 900$ K	83W2/LEED
	(2×1)O	Self-similar growth	89Z1/LEED+MCS
	(2×1)O	$T_c = 899$ K, 2D-Ising	85W1/LEED

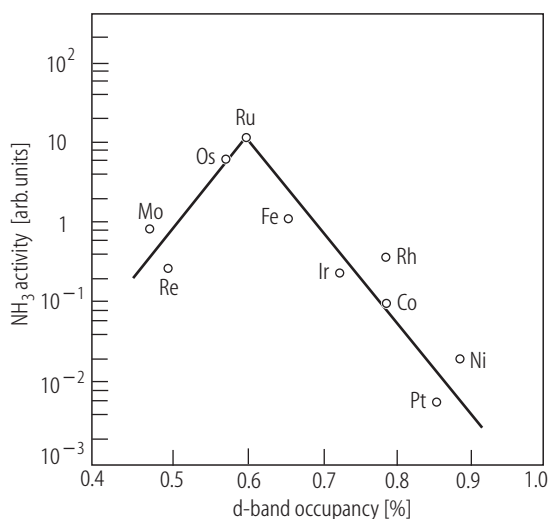
### 3.4.2.3 Nitrogen adsorption on metal surfaces

The interaction of atomic nitrogen with metal surfaces has been less intensely studied than that of oxygen. One reason might be that the high activation energy for dissociative adsorption of molecular nitrogen prevents easy production of atomic nitrogen adlayers on metal surfaces. The adsorption of atomic nitrogen and that of atomic oxygen is quite similar so that many general trends observed with O adsorption are equally found with atomic nitrogen.

The most common methods to deposit atomic nitrogen on transition metal surfaces are:

- 1) Atomization of  $N_2$  using high frequency discharge [77S1], a hot filament [66M1] or an ion gun [82R1].
- 2) Dissociative adsorption of hydrides of N ( $NH_3$  or  $N_2H_4$ ) followed by removal of the hydrogen by thermal desorption or by oxidation with pre adsorbed oxygen [81K4, 86B3, 89M2, 91W1]. This method is not as “clean” as method 1.
- 3) Dissociative adsorption of oxides of N (e.g. NO) followed by removal of the oxygen by reduction, and then thermal desorption of the reducing agent [91T1, 92C1].
- 4) Dissociation of NO by electron bombardment accompanied by electron stimulated oxygen desorption and following reduction of the residual oxygen by CO [93B3]. This method is not as “clean” as method 1.
- 5) Segregation of nitrogen (existing as impurity) from the bulk of the metal towards the surface. This effect was used with Cr(100) [97S4]. Other impurities in the bulk may segregate as well.

A major motivation in surface chemistry to study nitrogen adsorption on metal surfaces is coming from the ammonia synthesis, i.e. the production of  $NH_3$  from  $N_2$  and  $H_2$  (Haber-Bosch synthesis) [50M1, 94T2]. A good catalyst for ammonia should be able to dissociate molecular nitrogen without forming too strong bonds to the metal surface or without forming nitrides [80E1]. This interplay of trends renders Fe, Ru and Os good catalysts for ammonia synthesis (see Fig. 13). Investigations of nitrogen adsorption are also interesting for the formation of metal-nitrides. The development of metal nitrides poisons the activity of a metal surface towards ammonia synthesis; this is particularly true with Fe [87S1].



**Fig. 13.** The activity of various transition metals for ammonia synthesis is shown as a function of the degree of filling the d-band [81O2].

In general, the bonding of atomic nitrogen on metal surfaces is stronger than that of atomic oxygen (see Table 11). The main reason is that the valence states of N are so high that the coupling to the d states is strong enough to push anti-bonding states above the Fermi level. Although the N-metal bonding is strong, desorption temperatures are usually still quite low due to the strong internal bond of  $N_2$  (see Table 10).



The strong N-metal bond causes frequently local and global reconstructions of the metal surface. The hard sphere radius of adsorbed nitrogen is between 0.55 and 0.6 Å (see Table 14) which is close to the covalent radius of nitrogen (0.55 Å). Like oxygen, the chemisorbed N species is mostly covalently bound to the metal surfaces, as seen by typical XPS values of N(1s) appearing at about 397.6 eV. In the valence band region, the peaks characteristic for atomic nitrogen are located at about 5 eV below the Fermi level ( $E_F$ ). This energy position for the N(2p) derived emission from adsorbed atomic nitrogen is typical for most transition metals (see Table 12). Typical N against metal vibration are in the range 30 - 60 meV (see Table 13). Again similar to O the adsorbed N atoms are able to form ordered overlayers on the metal surfaces (see Table 15). However, since the binding energy and therefore the diffusion barrier of adsorbed nitrogen is higher than that of adsorbed oxygen, the ordering process of N is frequently kinetically hindered.

Due to the strong intra-molecular binding of N<sub>2</sub>, the dissociative sticking of N<sub>2</sub> is also very low, typical values of 10<sup>-6</sup> on Fe surfaces and 10<sup>-12</sup> on Ru surfaces (see Table 9). Both metals are particular active catalysts for ammonia synthesis [94T2].

### 3.4.2.3.1 The dissociative sticking coefficient of nitrogen on metal surfaces

**Table 9.** Sticking coefficient

Substrate	Surface	Sticking coefficient	Impact energy $E_i$ [eV]	Remarks	Method	Ref.
Fe(110)	initial	$1 \times 10^{-7}$		583 K - 733 K	TDS	77B2
		0	0.18 - 0.65	zero sticking for entropy reasons	Mol. beam	83B1
Fe(111)	initial	$6 \times 10^{-6}$		430 K; essentially no activation barrier, but a high entropy barrier	TDS/DFT	82E2, 77B3/99M1
		$10^{-6} \rightarrow 0.01^{a),c)}$	$0.25 \rightarrow 1$	e), direct molecular chemisorption (a-N <sub>2</sub> )	Mol. beam	87R1
		$1.2 \times 10^{-5}$		400 K - 580 K	TDS	97A1
Fe(100)	initial	$1 - 4 \times 10^{-7}$		380 K - 510 K		79E2, 82E1, 77B3, 76E1
Re(0001)	initial	$(9 \pm 2) \times 10^{-7}$		218 K, $E_{act} = 14 \pm 2$ kJ/mol	TDS	87H1
		$\sim 10^{-5}$			theory	90B3
Re(1120)	initial	$(4 \pm 1) \times 10^{-4}$		218 K, $E_{act} = 6 \pm 1$ kJ/mol	TDS	87H1
Ru(10 $\bar{1}$ 0)	initial	$< 10^{-12}$		RT; little N in subsurface	TDS	96D1
Ru(11 $\bar{2}$ 1)	initial	$< 10^{-12}$		RT; little N in subsurface	TDS	96D1
Ru(0001)	initial	$< 10^{-12}$		RT	TDS	96D1
		$< 10^{-3}$	1.25	sample 600 K	Mol. beam	96S4
		$5 \times 10^{-7} \rightarrow 10^{-2}$	$0.15 \rightarrow 4.0$	activation barrier: $\sim 2$ eV, dissociative sticking is achieved by $> 1.3$ eV	Mol. beam/DFT	97R1/97M3
W(110)	initial	0.003		300 K	TDS	79S1
		$< 3 \times 10^{-3} \rightarrow 0.35$	$0.31 \rightarrow 1$		Mol. beam (RT)	86P3, 84L1
W(111)	initial	0.08		300 K	KW	72K1
W(100)		$0.14 \rightarrow 0.4^{a),f)}$	$0.45 \rightarrow 5$		Mol. beam (300 K)	89R1
		0.63		340 K	TDS, KW	81B1, 74K1

- a) Initial adsorption probability increases with increasing kinetic energy
- a') Initial adsorption probability decreases with increasing kinetic energy
- c) Initial adsorption probability is surface temperature dependent
- e) Molecular intermediates detected after high kinetic energy exposure
- f) Initial adsorption probability decreases with increasing surface temperature

### 3.4.2.3.2 The heat of adsorption of chemisorbed nitrogen overlayers on metal surfaces

**Table 10.** Heat of Adsorption.

substrate	surface	heat of adsorption [kJ/mol]	activation barrier for desorption [kJ/mol]	Remarks/Method	Ref.
Ag(111)			106 and 130	Recombinative desorption	97C2
Cu(111)	<0.42 ML		143	recombinative desorption via the Cu(100)-c(2×2)N phase	98M3
	>0.42 ML		88		98S4
Fe(110)		212		TDS: 920 K, first order	77B3, 76E1
Fe(111)		203		TDS: 860 K, first order	77B2
Fe(100)		222		TDS: 980K, first order	77B3
poly-Fe	initial	167			51B1
	initial	293			55B1
Ir(111)		531			79E3
Ni(100)	initial	136			96V1
Re(0001)		601		recombinative desorption desorption energy: $(260 - 80\theta)$ kJ/mol, $0 \leq \theta \leq 1.0$	87H1 87G1
	(2×1)N	83		TDS, desorption at 580 K, isothermal desorption: $\nu_d = 2 \times 10^7 \text{ s}^{-1}$ $\nu_d = 2 \times 10^8 \text{ s}^{-1}$ $\nu_d = 2 \times 10^8 - 2 \times 10^{10} \text{ s}^{-1}$	92C1 93K1 92L1 98S6
Rh(110)	disordered	88			
	(2×1)N	107 - 120			
	(2×1)N	180			
Rh(111)	disordered	149		TDS, $\nu_d = 5 \times 10^{11} \text{ s}^{-1}$	93B3
Rh(100)		165		TDS, $\nu_d = 10^{11} \text{ s}^{-1}$	97J1
Rh(410)		100		TDS, $\nu_d = 10^7 \text{ s}^{-1}$	97J1
Rh(533)		70		TDS, $\nu_d = 10^7 \text{ s}^{-1}$	97J1
Re(0001)		487			90H1
Ru(10 $\bar{1}$ 0)		120		TDS	97D2
Ru(0001)		184		TDS	
		190		TDS	93S4
		112-120		TDS	93R1
poly-Ta	initial	575			50B1
poly-W	initial	397			51B1
W(110)	(2×2)N	648			71T1

**3.4.2.3.3 Nitrogen-metal bond strength (ab initio calculations)****Table 11.** The N-metal bond strength as computed by *ab-initio* calculations.

substrate	surface	N-metal bond strength	Ref./method
Ag(100)	initial	−14.5 kJ/mol (endotherm)	97R4/Cluster
Cu(100)	initial	230 kJ/mol	97R4/Cluster
Fe(110)	1/3 ML	135 kJ/mol (probably wrong structure)	99M1/DFT
	(2×1)N	550 kJ/mol w.r.t. atomic N	90R4/CEM
Fe(111)	( $\sqrt{3}\times\sqrt{3}$ )N	135 kJ/mol (probably wrong structure)	99M1/DFT
	(1×1)N	111 kJ/mol	
Fe(100)	c(2×2)N	234 kJ/mol	99M1/DFT
	c(2×2)N	572 kJ/mol w.r.t. atomic N (assumes the atomic geometry)	90R4/CEM
	(1×1)N	116 kJ/mol	99M1/DFT
Pd(111)	(2×2)-N	383 kJ/mol	98L1/DFT
	( $\sqrt{3}\times\sqrt{3}$ )-N	383 kJ/mol	
	c(2×2)-N	314 kJ/mol	
	( $\sqrt{3}\times\sqrt{3}$ )-2N	276 kJ/mol	
	(1×1)N	246 kJ/mol	
Pd(100)	(2×2)-N	407 kJ/mol	98L1/DFT
	c(2×2)N	362 kJ/mol	
	(1×1)N	169 kJ/mol	
Pt(111)	(2×2)N	415 kJ/mol	01M2/DFT
Rh(111)	(2×2)N	441 kJ/mol	98L1/DFT
	( $\sqrt{3}\times\sqrt{3}$ )N	446 kJ/mol	
	c(2×2)-N	408 kJ/mol	
	( $\sqrt{3}\times\sqrt{3}$ )-2N	371 kJ/mol	
	(1×1)N	303 kJ/mol	
Rh(100)	(2×2)-N	490 kJ/mol	98L1/DFT
	c(2×2)N	462 kJ/mol	
	(1×1)N	383 kJ/mol	
Ru(0001)	(2×2)N	561 kJ/mol	97S2/DFT
	(2×2)N	539 kJ/mol	
	(2×1)N	513 kJ/mol	
	(2×2)3N	475 kJ/mol	
	(1×1)N	436 kJ/mol	
W(110)	(2×2)N	617 kJ/mol w.r.t. atomic N	90R4/CEM
Zr(0001)	(1×1)N	409 kJ/mol, N-octahedral between 2. and 3. Zr layer	97Y1/DFT

Remark:

Cluster calculations produce less reliable values for N-metal binding energies than slab calculations.

### 3.4.2.3.4 Electronic properties of chemisorbed nitrogen on metal surfaces

**Table 12.** Electronic properties of chemisorbed atomic nitrogen overlayers on metal surfaces.

substrate	surface	Binding energies of core and valence states	Ref.
Ag(111)		N(1s): 397.9 eV, UPS: 3.4 eV, 8.2 eV	77G2/XPS, UPS
Cr(110)	10 L N <sub>2</sub>	At room temp.: surface nitride; shift of the peak at 41.5 eV	84M1/EELS
Cr(111)		N(1s): 397.8 eV	88F1/XPS
Cr(100)	(1×1)N	N(2p): 2.5, 4.7 eV disperse strongly by 2 eV, 1 eV	80G3/ARUPS
Cu(110)	(2×3)-3N >0.5 ML	N(1s) 396.5 eV N(1s): 396.5, 397.2 eV a second N species on 4-fold site	90B2/XPS
Cu(100)	c(2×2)N	N(2p): 1.2 eV, 5.6 eV below $E_F$ N(1s): 396.3 eV	77T1/UPS 77T1/XPS
	low N coverage	N(2p <sub>z</sub> ), N(2p <sub>x,y</sub> ) separated	98W3/SXES, XAS
	low N coverage	Calculated XAS, XES N(1s) spectra	98T3/cluster
	c(2×2)N	N K emission: 391.4, 396 eV and 390.3, 393.2, 395.2, 397 eV: strong 2p-4sp bonding state, strong 2p-3d antibonding state	94W1/SXES
	c(2×2)N c(2×2)N	N(1s): 396.4 eV N(2p): 1 eV, 6 eV below $E_F$	90N1/XPS 94W1/UPS
Fe(111)		N(2p): 5 eV, 1.8 eV	77B3
		N(1s): 397.5, 397.0 eV on- and sub-surface nitrogen	87A3/PES
Gd(0001)		N(2p <sub>z</sub> ): 5.6 eV, N(2p <sub>x,y</sub> ): 3.4 eV	95W3/PES
Ir(110)		NO dissociation; atomic N: N(1s): 398.14 eV	00D1/XPS
Ni(100)	(2×2)N	−1.0, −3.5 eV above $E_F$ , probably due to hybridization of N(2p) with Ni(d), KRIPES: flat dispersion.	94H1/ IPE
	(2×2)p4g-N	N K emission: 391.6 eV, 397 eV: 2p-4sp bonding state; weak 2p-3d antibonding state	94W1/SXES
	(2×2)p4g-N	N(1s): 397.3 eV	90N1/XPS
	(2×2)p4g-N	N(2p): 1.5, 5 - 6 eV below $E_F$	89K1/UPS
Re(0001)	(2×2)N	5 eV	89H1/ELS
Rh(110)	(2×1)N	dispersion of N(2p <sub>y</sub> ) along Rh-N chains (y-direction) from 5.4 to 6.3 eV, no dispersion perp. to Rh-N rows.	95D1/ ARUPS
Ti(0001)	1 - 1000 L	300 K: N(1s): 397.3 eV (octahedral), 395.8 eV (on-surface)	97F1/XPS
	1 - 1000 L	200 K: N(1s): 398.2 eV (on-surface), 397.3 eV (octahedral)	97F1/XPS
	1 - 1000L	473 K: N(1s): 397.3 eV (octahedral), 397.8 eV (dissolved), 395.8 eV (on-surface)	97F1/XPS
W(110)	(2×2)N	N(2p) 6 eV below $E_F$	79S1/UPS

### 3.4.2.3.5 Vibrational properties of chemisorbed nitrogen atoms

**Table 13.** Vibrational properties and suggested adsorption sites of (atomic) nitrogen overlayers on metal surfaces. If not otherwise indicated the technique of HREELS or IRAS was used.

substrate	structure	Me-N stretch vibration [meV]	adsorption site	Ref.
Cr(111)		67	3-fold	88F1
Cr(100)	initial	70	2-fold	85B3
Cu(110)	(2×3)-N (2×3)N	50 10.5, 45.5, 54.5, 68.0, 45.5, 68.0, 82.0, 82.0, 86.5, 71.5, 48.5, 84.5	quasi-5-fold N-modes confirmed by theory	88H1 96H2
Cu(111)	distorted Cu(100)-c(2×2)	34.5, 50.5	4-fold	86H1
Cu(100)	c(2×2)N	40.5, 94 perpendicular Cu-N	4-fold	87M4
Fe(111)	-	56	-	84G1, 85T2
Fe(100)	c(2×2)N	61	4-fold	90L2
Ni(110)	(2×3)-N	24, 46	long-bridge	88K1
Ni(100)	(2×2)p4g-N	89.0 - 92.5 (parallel mode) 34 - 54 (perpendicular) Rayleigh mode temperature dep.	reconstruction	86D1
Pd(110)	(2×3)-N	32 55 90 130	long-bridge long-bridge short-bridge on-top	87K1
Rh(110)	(2×1), (3×1)	56	long-bridge	92C1
Re(0001)		46	3-fold	90H1
Ru(10 $\bar{1}$ 0)	0.6 ML (-1,1,2,1)-N	60 (perp.), 41 (lateral)	hcp-sites	97D2
Ru(0001)	(2×2)N ( $\sqrt{3}\times\sqrt{3}$ )N (2×2)N	72 (perpendicular)  67 (perp.), 63 (lateral)	hcp site  hcp site	93S1  97M3/DFT
W(110)	(4×1)N	90 ( $\beta_1$ -TD peak) 60 ( $\beta_2$ -TD peak)	- -	89S2
W(100)	c(2×2)N	60	4-fold hollow	80H1

### 3.4.2.3.6 Local atomic nitrogen-metal geometry

**Table 14.** The N-metal bond length and other structural characteristics.

substrate	surface	N-metal [ $\text{\AA}$ ]	Adsorption site/Remarks	Ref./Method
Ag(100)	initial	2.12	4-fold	97T1/Cluster
Cr(100)-2Co	(1 $\times$ 1)N	2.04, 1.94	deep in hollow site of bcc Co bilayer	93S3/LEED
Cr(100)	(1 $\times$ 1)N	2.04, 2.02	deep in hollow site	89J1, 92J1, 97R5/LEED
	c(2 $\times$ 2)N	2.07, 1.97	deep in hollow site	98S5/LEED, STM
Cr(110)	( $\sqrt{6}\times\sqrt{6}$ )R35°	-	N-induced herringbone reconstruction	97S4/STM
Cu(110)	(2 $\times$ 3)-4N		quasi-5-fold, square reconstruction	90A2/LEIS
				90R1/PhD
				91S2/NICISS
		1.83, 2.12		93B5/SXRD
		1.87, 1.88		94V1, 97M1/LEED
Cu(111)	LT 500 K	-		96W1/SEXAFS
		1.81		91D3/EXELFS
			disordered N	98S4/STM
			Cu(100)-c(2 $\times$ 2)N	
Cu(100)	c(2 $\times$ 2)N	1.81, 1.95	N: deep in 4-fold hollow site	87Z1/LEED
	c(2 $\times$ 2)N	1.85, 2.29	N-Cu co-planar, lower symmetry	93L2/SEXAFS
	c(2 $\times$ 2)N	1.77		01H1/PhD
	c(2 $\times$ 2)N	-	Vertical rumpling of 0.34 $\text{\AA}$	01D3/PhD
	initial	1.87	-	97T1/Cluster
		1.84	-	91D3/EXELFS
Fe(110)	0.5 ML		Fe(100)-c(2 $\times$ 2)N like overlayer	99M1/DFT
Fe(111)	0.5 ML		Fe(100)-c(2 $\times$ 2)N like overlayer	99M1/DFT
Fe(100)	c(2 $\times$ 2)N	1.81	4-fold	82I1/LEED
	c(2 $\times$ 2)N	1.90	4-fold	99M1/DFT
	(2 $\times$ 2)N	1.96	4-fold, no experiment	99M1/DFT
	(1 $\times$ 1)N	1.85	4-fold, no experiment	99M1/DFT
Mo(100)	c(2 $\times$ 2)N	2.45, 2.60	4-fold	75I1/LEED
Ni(110)	(2 $\times$ 3)-3N	1.86 $\pm$ 0.03	N hollow, square reconstruction	94W1/SEXAFS
Ni(111)		-	N-hollow at room temperature Ni(100)-c(2 $\times$ 2)N like structure after annealing at 670 K	93O2/NEXFAS
Ni(100)	(2 $\times$ 2)p4g-N	1.89	deep in 4-fold site, clock reconstruction type 1	87W1/SEXAFS
	(2 $\times$ 2)p4g-N	1.85		91K1/PhD
	(2 $\times$ 2)p4g-N	1.85		99A1/DFT
	(2 $\times$ 2)p4g-N	-	lateral displacements of topmost Ni atoms by 0.3 $\text{\AA}$	99D2/SXRD
Pd(111)	( $\sqrt{3}\times\sqrt{3}$ )N	1.94	fcc (assumed)	98L1/DFT
Pd(100)	c(2 $\times$ 2)N	2.07	4-fold	98L1/DFT

substrate	surface	N-metal [ $\text{\AA}$ ]	Adsorption site/Remarks	Ref./Method
Rh(110)	(2 $\times$ 1)N	1.87 $\pm$ 0.08 1.94 $\pm$ 0.08	long-bridge, missing row	95G2, 95D1/LEED
Rh(111)	( $\sqrt{3}\times\sqrt{3}$ )N	1.95	fcc (assumed)	98L1/DFT
Rh(100)	c(2 $\times$ 2)N	2.07	4-fold	98L1/DFT
		2.03	4-fold	99A1/DFT
Ru(0001)	(2 $\times$ 2)N	1.93 $\pm$ 0.05	hcp	97S2/LEED
	( $\sqrt{3}\times\sqrt{3}$ )N	1.93 $\pm$ 0.06	hcp	97S2/LEED
	(2 $\times$ 2)N	2.00, 1.98	hcp	97S2, 97M2/DFT
	( $\sqrt{3}\times\sqrt{3}$ )N	1.97	hcp	97S2/DFT
Ti(0001)	(1 $\times$ 1)N	2.10	N underlayer, octahedral	76S1/LEED
	1-1000L at RT	-	N-octahedral and on-surface	97F1/XPD, XPS
W(110)	(2 $\times$ 2)	-	N-underlayer	79S1/ISS
W(100)	<0.5 ML	1.67, 1.87	-	98O4/EELFS
W(100)	c(2 $\times$ 2)N	2.28, 2.13	deep in 4-fold site 0.27 $\text{\AA}$ buckling in the 2. W-layer	95B1, 82G2/LEED
Zr(0001)	(1 $\times$ 1)N	2.27	N underlayer	87W1/LEED
		2.27	N-octahedral	97Y1/DFT

### 3.4.2.3.7 Ordered overlayers of chemisorbed nitrogen atoms on metal surfaces

**Table 15.** Ordered overlayers of chemisorbed nitrogen on metal surfaces. If not otherwise indicated the technique of LEED was used. No structure determination.

Substrate	Orientation	N-surface structure	Ref./Method
fcc-Cu	(110)	(2 $\times$ 3)	94V1
		(2 $\times$ 3)	98T4/STM
	(111)	Pseudo (100) reconstruction	99D1/STM
	(100)	c(2 $\times$ 2)	76B1
		c(2 $\times$ 2)	01D2, 01E1/STM
bcc-Fe	(110)	2 phases, reconstruction	77B2
	(211)	(2 $\times$ 5)	97H2
	(111)	4 phases c(2 $\times$ 2), (3 $\times$ 3) reconstruction	77B3
		(3 $\sqrt{3}\times 3\sqrt{3}$ )R30°, (5 $\times$ 5)	97A1
	(100)	c(2 $\times$ 2) initial adsorption of nitrogen	82I1 00P1/STM
fcc-Ni	(110)	(2 $\times$ 3)	82R1
		(2 $\times$ 3)	96T2, 93V2/STM
	(111)	c(5 $\sqrt{3}\times 9$ )rect., “(2 $\times$ 6)”	93G3
	(100)	(2 $\times$ 2)p4g	93L3/STM
fcc-Pd	(110)	(2 $\times$ 3)	88K1
	(100)	c(2 $\times$ 2)N	90Y1, 91Y1
fcc-Rh	(110)	(2 $\times$ 1), (3 $\times$ 1)	92C1
	(111)	disordered	92B1
	(100)	c(2 $\times$ 2)	91T1



Substrate	Orientation	N-surface structure	Ref./Method
hcp-Re	(0001)	(2×2)	89H1
hcp-Ru	(0001)	(2×2), ( $\sqrt{3}\times\sqrt{3}$ )R30°	94B1
hcp-Ti	(0001)	(1×1)N underlayer	76S1
bcc-W	(100)	c(2×2)	68O1
bcc-W	(110)	(2×2), N underlayer	79S1

### 3.4.2.4 Carbon adsorption on metal surfaces

The interaction of atomic carbon with metal surfaces has been even less intensely studied than oxygen and nitrogen, mainly because the preparation of pure carbon layers is more involved. The preparation of carbon overlayers requires the dissociation of carbon containing molecules, such as  $C_2H_2$ , CO,  $C_2H_4$  etc., leading to coadsorption. In order to end up with a pure carbon overlayer, the other constituents, such as oxygen and hydrogen, have to be removed from the surface. Another popular procedure to produce C-overlayers on metal surfaces is segregation of carbon from the bulk.

Carbon is able to form carbidic carbon (isolated adsorbed C atoms) and graphite overlayer on metal surfaces. Only the carbidic carbon is desired in catalytic reaction. Graphite layers are considered to poison the catalytic activity of metal surfaces. CO and  $H_2$  can be catalyzed to form  $CH_4$  and higher alkanes together with water [82B1]. This process requires as the rate determining step the dissociation of CO on the catalyst's surface. If the C-O bond is preserved, the reaction with  $H_2$  results in products containing oxygen, such as alcohols. For the catalytic CO hydrogenation reaction Sabatier was awarded with the Nobel Prize in chemistry 1912 [12S1].

The binding mechanism of carbidic carbon to metal surfaces is similar to that of oxygen and nitrogen. This is reflected in the electronic properties (see Table 17) where about 5 eV below the Fermi energy C(2p) derived states are observed. Typical C against metal vibrations reveal energy losses of about 50 - 60 meV (see Table 18). The bond strength determined by ab-initio calculations is about 6 eV (see Table 16). The resulting hard sphere radius of carbon on metal surfaces (determined by the carbon-metal bond length minus the half of the metal-metal bond length) is about 0.55 Å which is substantially smaller than typical O and N hard sphere radii of about 0.70 Å and 0.65 Å, respectively; for C-metal bond length the reader is referred to Table 19. However, due to the smaller size of carbon in comparison to oxygen and nitrogen, carbon atoms can easily penetrate the topmost metal layer.

Quite in contrast, a graphite overlayer is characterized by a very strong internal C-C binding energy and a weak interaction to the metal surface. Due to the strong C-C bonding, graphite forms always a hexagonal overlayer regardless of the symmetry of the metal surface. Carbidity carbon, on the other hand, is able to form ordered structures as manifested in Table 20.

Many physical-chemical quantities cannot be measured. For instance, the sticking coefficient of carbon does not make sense, since the formation of carbon on a metal surface requires several reaction steps on the surface such as with the dissociation of  $C_2H_2$  or CO and other C containing products. The same problem is encountered with the heat of adsorption. Therefore sticking coefficients and experimentally determined heats of adsorption are not presented for carbon.

The interaction with C is also important for studying the formation of metal carbides, diamond films, nano-tubes and  $C_{60}$  molecule.

### 3.4.2.4.1 Carbon-metal bond strength

**Table 16.** The C-metal bond strength as computed by *ab-initio* calculations.

substrate	surface	C-metal bond strength [kJ/mol]	Me-C bond length [Å], adsorption site	Ref./method
Co(0001)	(2×2)C	680	1.79, hcp	98K3/DFT
	(2×2)C	646	1.85, subs.	
	1 ML C	530	1.84, hcp	98K3/DFT
	1 ML C	655	1.90, subs.	98K3/DFT
Cu(111)	single C	296		97L1/cluster
Fe(100)	single C	656	2.17	93B4/cluster
Ni(111)	single C	743	3-fold hollow	97L1/cluster
	(2×2)C	589	fcc	00W2/DFT
	(2×2)C	644	1.89, fcc	98K3/FP-LAPW
	(2×2)C	708	1.86, subs.	
	1 ML C	480	1.89, fcc	
	1 ML C	589	1.91, subs.	
		608		98B1/DFT
	(1×1)C	728		74S1/ESS
Ni(100)	(2×2)C	690, 713		75I1/ESS
Pd(111)	single C	614	3-fold hollow	97L1/cluster*
Pt(111)	(2×2)C	526		97M1/DFT
	single C	651		97L1/cluster

Remarks

- a) \*be careful: for oxygen on the same surface the authors favored on-top adsorption!  
 b) Cluster Calculations produce less reliable values for C-metal binding energies than corresponding slab calculations.

### 3.4.2.4.2 Electronic properties of chemisorbed carbon on metal surfaces

**Table 17.** Electronic properties of chemisorbed atomic carbon overlayers on metal surfaces.

Substrate	Surface	State	Binding energy [eV]	Remarks	Ref./Method
Co(100)	(2×2)-C		273	fcc-Co(100): carbidic C	78M4/AES
Cu(110)			272	Carbidic C	87S2/AES
			288, 295	C K-edge	87S2/EELS
Cu(100)			272	Carbidic C	87S2/AES
			281, 288, 295	C K-edge	87S2/EELS
Fe(100)	c(2×2)-C	C(2p)	3.0		77R3/UPS
	c(2×2)-C	C(2p), Fe(3d)	-2.5, -3.9	antibonding states	92H2/IPE
Ir(110)	contamination	C(1s)	284.5		97L2/XPS
Mo(110)	(4×4)	C(1s)	273		92H3/AES
Mo(001)	(1×1)C	C(1s)	283	Carbidic C	76G1/XPS
		Mo	225.5, 229.5		

Substrate	Surface	State	Binding energy [eV]	Remarks	Ref./Method
Ni(110)	(4×5)	C(2p)	~4	Carbide C disperses from 6 eV to 6.5 eV, from 4.2 eV to 5.2 eV	85P1/UPS
	(2×1)-C	C(2p)			91P3/PES
	(2×2)C	C(2p)			86M1/ARUPS
N(111)	0.2 ML		1.0, 4.2, 13.0		83R2/PES
Ni(100)	(2×2)C		-1.5 - -2	probably hybridization of O(2p) with Ni(d), KRIPES: flat dispersion. C(2p) derived state disperses from 3.4eV to 4.6eV	94H1/IPE
	(2×2)C				86P2/ARUPS
	(2×2)-C	C(2p)	4.0, 6.0	C KVV	82K2/UPS
		C(2s)			91H2, 91H3/AES
	(2×2)-C		282.9		91N1/XPS
	(2×2)p4g-C	C(1s)	282.9		94Z2/XPS
	(2×2)p4g-C	Ni(2p <sub>3/2</sub> )	853.2		
Re(0001)	7×√19	C(1s)	273		72Z2/AES
Rh(111)	C + O coadsorption		5.2, 9.4, 11.5		89K1/UPS
Ru(0001)	Carbon	C(s,p <sub>z</sub> ) derived	9.8		82H1/UPS
W(100)	0.5-1.0 ML	C(2p)	4.8	several peaks	84J1/UPS
	0.1-1.0 ML	W(4f <sub>7/2</sub> )	31 - 32		95L3/HRCLS

#### 3.4.2.4.3 Vibrational properties of chemisorbed carbon atoms

**Table 18.** Vibrational properties of (atomic) carbon overlayers on metal surfaces. If not otherwise indicated the technique of HREELS or IRAS was used.

Substrate	Structure	Me-C stretch vibration [meV]	Remarks	Adsorption site	Ref.
Cr(111)		55, 71	dissociation of CO, 0.5 L CO	3-fold, 2-fold	86B5
Cr(110)		53, 70	dissociation of CO, 0.2 L CO	3-fold, 2-fold	86B5
Cr(100)	low coverage	65	dissociation of CO	4-fold	85B3, 86B5
Fe(111)		51		3-fold	86B2
Fe(100)	c(2×2)C	54		4-fold	90L2
Ni(100)	disordered (2×2)p4g-C	50	(<0.3 ML) perpendicular	clock-wise reconstruction	87R2, 89S3
		42.5	perpendicular mode		
		87.5 - 90.6	parallel mode		

**3.4.2.4.4 Local atomic carbon-metal geometry****Table 19.** The C-metal bond length and other structural characteristics.

Substrate	Surface	C-metal [ $\text{\AA}$ ]	Adsorption site/Remarks	Ref./Method
Al(111)	C disordered low C cov.	-	hcp!	90B3, 92B2, 95F2
Al(100)		2.1	4-fold	86M1/cluster
Co(0001)		1.75	hcp	87A1/LEED
	(2×2)C	1.79	hcp	98K3/FP-LAPW
	(2×2)C	1.85	substitutional	
	1 ML C	1.84	hcp	
	1 ML C	1.90	substitutional	
Fe(111)	cluster	-	C-underlayer	91A1/cluster calc.
Fe(100)	c(2×2)C+O	2.09, 1.92	4-fold	78J2/LEED
Mo(100)	low C cov.	-	4-fold, no reconstruction	83O1/LEIS
	c(2×2)C	2.28, 2.17	deep in 4-fold site	95J2/LEED
Mo(111)	small amounts of C	-	upon annealing C penetrates the region (5 $\text{\AA}$ below the surface)	87O1/LEIS
Ni(110)	(2×1)C	1.85	3-fold in troughs	91C2/EELFS
Ni(111)	(2×2)C	1.89	fcc	98K3/FP-LAPW
	(2×2)C	1.76	fcc	00W2/DFT
	(2×2)C	1.86	substitutional	98K3/FP-LAPW
	1 ML C	1.89	fcc	98K3/FP-LAPW
	1 ML C	1.91	substitutional	98K3/FP-LAPW
Ni(100)	(2×2)p4g-2C	1.82, 1.95	deep in 4-fold site, clock reconstruction type 1	91G1, 79O1/LEED
	(2×2)p4g-2C	1.85, 1.99		91K1/PhD
	(2×2)p4g-2C	1.85		87B1/SEXAFS
	(2×2)p4g-C	1.85		89A2/SEELFS
	0.15 ML	1.87, 1.99	undistorted 4-fold site	99A1/DFT
		1.79, 1.94		99T1/PhD
Rh(100)	c(2×2)-2C	2.01	no clock reconstruction	99A1
W(100)	(1×5)4C	C-W layer distance: 0.5 $\text{\AA}$	4-fold hollow O-coadsorption drives C into the subsurface region	88M1/LEIS 89M1/AES, LEIS
	( $\sqrt{2}\times\sqrt{2}$ )R45°	-	surface reconstruction	95L3/HRCLS
Zr(0001)	(1×1)C	2.29	C-underlayer, octahedral	88W1/LEED

### 3.4.2.4.5 Ordered overlayers of chemisorbed carbon atoms on metal surfaces

**Table 20.** Ordered overlayers of chemisorbed carbon on metal surfaces.

Substrate	Orientation	N-surface structure	Ref.
fcc-Co	(100)	p(2×2)C	78M4
hcp-Co	(1120)	(2×5)	98V1/STM
bcc-Fe	(100)	c(2×2)	90L2
bcc-Mo	(100)	(1×1)C	80K1
	(100)	(4×4)C; $\alpha$ -Mo <sub>2</sub> C(0001)	91Y1
	(110)	(2×1), (1×2)	76G1
		(4×4)	92H3
fcc-Ni	(110)	(4×5)pmg	85P1
	(100)	(2×2)p4g, splitted c(2×2)	79O1, 87B1, 87R2
	(100)	clock reconstruction	94H3/STM
	(997)	clock reconstruction	00N1/STM
	(111)	(1×1)2C, graphitic C	83R2
		c(5√3×9)rect	93G3
		(√39 × √39)R16.1°	89N2
hcp-Re	(0001)	7×√19	72Z2
bcc-W	(100)	c(2×2)-2C, c(3×2)-4C, (5×1)-4C	73L1, 84J1, 89M1
	(110)	R(15×12)	68B1/LEED
		R(15×3)	95B8, 96B6/STM
hcp-Zr	(0001)	(1×1)C underlayer	88W1

**3.4.2.5 References for 3.4.2**

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