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Book Review

Surface Crystallographic Information Service, A Handbook of Surface Structures (Edited by J.M. MacLaren, J.B. Pendry, P.J. Rous, D.K. Saldin, G.A. Somorjai, M.A. Van Hove and D.D. Vvedensky), D. Reidel Publishing Company, Dordrecht, Boston, Lancaster, Tokyo, 1987, vii + 352 pages, DFl 165, $79, £56. ISBN 90-277-2503-9.

The Handbook of Surface Structures has been designed to provide "all those whose work involves surfaces" with an easy means of accessing reported structural data for both clean and adsorbate-covered surfaces. With such a wide target audience, this compendium must aim to satisfy the expert in the field, the novice to the field, and those who neither claim nor wish to be surface scientists, but who nevertheless need a specific piece of structural information. The coordination chemist is likely (though not without exception) to fall into the last category, possibly wanting data on substrate-adsorbate bond lengths or adsorbate structures without the prospect of spending hours in a library floundering through a mass of ambiguously worded reports that are crowded with synonyms and undefined sign conventions.

This handbook contains information on one hundred and ninety-six surface structures arranged primarily by the atomic number of the principal substrate atom, then (in diminishing order of precedence) by decreasing density of the surface plane, by increasing atomic number of the pricipal adsorbate atom and by increasing complexity of the surface mesh. However, the "fringe" surface scientist may well find the alphabetic lists of common names {*e.g.* Si(111) (2x1)} and author's names a more amenable route to material of interest. The handbook incorporates seventy-one figures depicting, in addition to the 'standard' structures, those structures for which a written description would be inadequate or over complicated. The quality of the Figures is excellent although the perspective chosen for some of them will undoubtedly require familiarization.[†] The example overleaf shows a typical Table and its associated Figure. As can be seen the computer generated text is rather hard to read (boxed entries would have been clearer) but at least the Greek characters and symbols such as ✓ and ° appear correctly - which cannot be said of the index where ✓ appears as {, ° appears as x, and α is represented by an apostrophe!

[†] The handbook is complemented by a software package (ISBN 90-277-2504-7) for IBM PCs which enables new structural data to be added and visualized; this will be reviewed at a later date.

COMMON NAME: Cu(110) HCO2-DISORDERED
CLASSIFICATION: 29.6.1.8.3
DATE OF FIRST PUBLICATION: 28 JAN 1985
REFERENCE:
A PUSCHMANN J HAASE MD CRAPPER CE RILEY AND DP WOODRUFF, PHYS REV LETT VOL 54 2250 (1985)
DATE ENTERED IN SCIS: JUNE 1986
SURFACE:

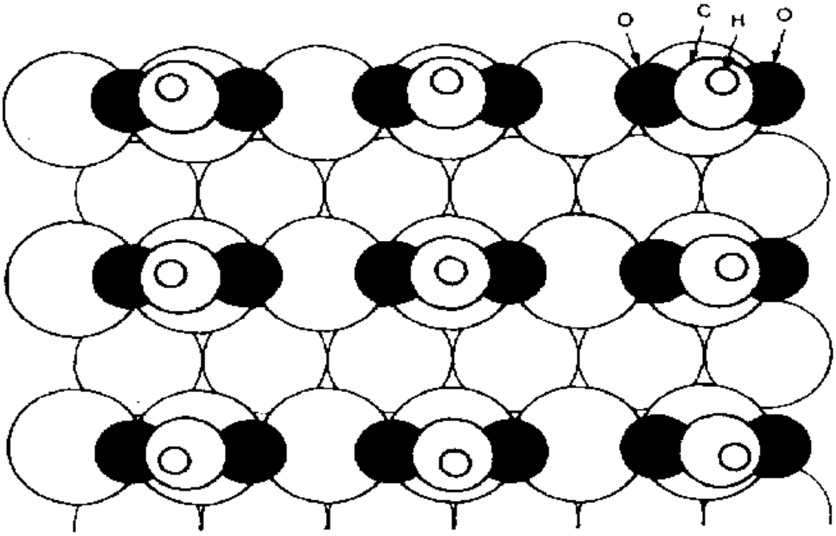
SUBSTRATE	FACE	ADSORBATE	SURFACE PATTERN
Cu	(110)	HCOOH	DISORDERED
BULK STRUCTURE	TEMP	ADS STATE	COVERAGE
FCC	300K	HCO2(FORMATE)	

STRUCTURE:
REFERENCE UNIT CELL a=5.12 b=3.62 A(a,b)=90

LAYER	ATOM	ATOM POSITIONS		NORMAL LAYER SPACING	ERROR
A1	C	0.5	0.0	0.53	
A2	O	0.721	0.0	0.0	
A3	O	0.279	0.0	1.51	
S1	Cu	0.0	0.0	0.0	
S2	Cu	0.5	0.0	1.28	
S3	Cu	0.25	0.5	0.0	
S4	Cu	0.75	0.5	1.28	

2D SYMMETRY	THERMAL VIBRATIONS	R(-)
-	-	-

SURFACE PREPARATION:
FORMATE SPECIES FORMED BY EXPOSURE TO FORMIC ACID AT ROOM TEMPERATURE.
CLEANLINESS:
-
METHOD OF STRUCTURAL DETERMINATION:
NEXAFS WITH EMPIRICAL CORRELATIONS TO GET C-O BOND LENGTH AND O-C-O BOND ANGLE, SEXAFS WITH COMPARISON OF CALCULATED AND MEASURED AMPLITUDES FOR DIFFERENT POLARIZATION ANGLES TO GET ADSORPTION SITE.
EXPERIMENTAL DATA:
NEXAFS OF O KLL AUGER LINE WITH POLARIZATION ALONG [1-10] AND [001] AZIMUTHS AT NORMAL AND GRAZING INCIDENCE, SEXAFS OF O K EDGE WITH SIMILAR POLARIZATION ORIENTATIONS.
STRUCTURES EXAMINED:
FORMATE PLANE PERPENDICULAR TO THE SURFACE ALONG [1-10] AZIMUTH WITH OXYGENS POINTING TOWARDS THE SURFACE AND CARBON ATOM OVER A TOP OR BRIDGE SITE, H IGNORED.
COMMENTS:
Cu-O BOND LENGTH DETERMINED BY SEXAFS IS AN AVERAGE OF TWO UNEQUAL LENGTHS(1.88 AND 2.08A).
RESULT IS HCO2 SPECIES WITH TWO OXYGENS OVER TWO ADJACENT SHORT BRIDGE SITES (OFF-CENTER TOWARD EACH OTHER), C BRIDGING THE TWO OXYGENS IN A PLANE PERPENDICULAR TO THE SURFACE (H ASSUMED PERPENDICULARLY ABOVE C).
SEE FIGURE S46



Cu (110) HCO_2

The editors hope that "as the compilation expands with time .... it will become one of the standard reference works for structures: in the manner of Wyckoff and other X-ray tables are for bulk crystals". This is an admirable target for the future, but unfortunately this first edition falls way short. For such a compilation to be a useful source book it should be comprehensive, accurate and easy to use; this book fails, to varying degrees, on all three counts.

Comprehensiveness. The listing is obviously incomplete, to an unknown extent, because the editors have made a *selective* choice of structures. Some of the criteria for inclusion are stated in the introduction, but the application of these criteria appears to be peculiarly subjective. For instance, the structures of tellurium and iodine adsorbed on Si(111) are included, but the structures of the same adsorbates on Ge(111) - reported in the same paper - are not! It is impossible to tell whether the missing structures have been omitted inadvertantly, or because they are incorrect in some way, or because they violate the editors' incorporation criteria in some way. The inclusion of lists of structures deemed unsuitable for full tabulation and the reason for their rejection would require little extra effort (the papers have to be read anyway) and would remove these uncertainties. The editors' *have* clearly violated their own criteria by inclusion of some of their own *unpublished* observations.

Accuracy. Unfortunately it is all too easy to find errors in this book. Despite (or perhaps because of) its team of seven editors, the cross-checking and proof-reading appears to have been at best half-hearted. There are numerous spelling mistakes in obvious places (such as authors names), and many other inconsistencies in the classification of structures (such as incorrect atomic numbers, format mistakes, *etc.*). Such comments may seem petty and nitpicking, but accuracy is particularly important in data compilations; errors in the words are an inevitable indicator of errors in the numbers - much less easy to spot at first glance. More importantly, perhaps, there are major errors in the descriptions of experiments (especially those not using low energy electron diffraction - LEED) and readers would be very ill-advised to use this book without checking the original papers.

Ease of use. The compilers have tried to include all the structural information needed to specify each structure. However the format they have chosen is dominated by the ideas of LEED, where the perpendicular inter-layer spacing is a key variable. The coordination chemist interested in chemical trends (such as bond length/bond order relationships) would find this book difficult to use. Adsorbate-substrate bond lengths are not given in most cases {*e.g.* Cu(100)c(2x2)Cl}, even when the structure was solved by SEXAFS (where this parameter is the primary quantity determined). In addition, the adsorption site is not stated for some bridge structures, and it can be very difficult to deduce.

If the errors are corrected and more structures are included, together with information on rejected structures, the next edition of this book will be worth buying; however, this first edition cannot be recommended other than as a starter - back to the library, chaps!

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