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The NIST Surface Structure Database - SSD Version 4

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ABSTRACT

SSD-4, the fourth version of the NIST Surface Structure Database is to appear in early 2002 as a significant upgrade to both the database and graphics software; it now also includes nearly 1300 structures published through the end of 2000. SSD is an interactive PC-based database of critically-selected surface structures determined with a variety of experimental techniques. The data include not only atomic coordinates, bond lengths and bond angles, but also information about experimental preparation, measurement and analysis methods. The software provides advanced search and display facilities, as well as interactive three-dimensional color visualization and analysis tools of great flexibility. In addition, the program can generate publication-quality color or gray-scale prints of any structure, with a host of user-selectable options (such as view angle, perspective, colors, ball and bond styles, and labels).

1. OVERVIEW OF SSD

The NIST Surface Structure Database (SSD) provides extensive information about critically selected surface structures determined from experiment. A unified format is used to allow convenient direct comparisons of related but different structures, or of results obtained with different techniques for the same structure. Powerful tools are available for searching the database and for the graphical visualization and analysis of individual structures. The criteria for inclusion of structures in the database are

- publication or acceptance in refereed journals or proceedings;
- determination with proven techniques and analysis methods;
- reasonable completeness of the structure determination;
- complete description of the structure.

SSD includes

- commensurate structures (which covers most solved structures);
- incommensurate structures (formed for instance by physisorption);
- disordered structures of adsorbates and alloys;
- solid-solid interfaces.

Figures 1-3 show the types of surface structures included in SSD-4 [1]. Figure 1 counts structures by the kind of substrate material, categorizing three different criteria: elemental vs. metallic alloy vs. other compound; metal vs. semimetal vs. semiconductor vs. insulator; and non-reconstructed vs. reconstructed. Figure 2 counts structures by the lattice type of the substrate (whether clean or adsorbate-covered): fcc, bcc, etc. Figure 3 counts structures by the type of adsorbate structure: atomic vs. molecular vs. compound adsorption; substitutional vs. interstitial adsorption; adsorption as an overlayer; and pseudomorphic vs. other epitaxial multilayer growth. These counts reflect the emphasis of past research on simple metal surfaces and a few semiconducting materials; however, the new structures added to SSD-4 (not specifically shown in the figures) continue a clear trend toward more diverse and more complex surface structures [2,3].

Figure 4 shows a typical initial display of data for a particular structure chosen from the database. It consists of two main windows: a summary window at left and a graphics window at right. A structure list is also shown at the bottom right, from which this particular structure was selected. At bottom left are five data buttons, which allow other windows to be opened to display further information about this structure. For instance, an experiment/theory window can be opened, shown in Figure 5, that gives details about sample preparation, data collection, theory/data treatment, structures examined, and quality of experiment/theory fit. Other windows provide information about the two-dimensional unit cells present in the structure, the coordinates of individual atoms, and a selection of bond distances and bond angles.

There are three modes of use of SSD-4: browsing, searching, and comparing. Individual records in the database can be viewed along with the associated three-dimensional picture of the structure by browsing from record to record, as displayed in Figure 4. More usefully, sets of related structures can be found by searching the database. Three-dimensional pictures of up to

three structures can be simultaneously displayed and analyzed in the compare mode: the latter two modes will be briefly described and illustrated in the next two sections, while another section will cover the three-dimensional visualization and analysis capabilities of SSD-4.

2. SEARCHING FOR STRUCTURES

Subsets of related structures can be extracted from the full database using a simple search process. Search criteria are typed, or selected from drop-down lists, in the search criterion form, as illustrated in Fig. 6.

The selection criterion shown in Fig. 6 will select those structures of reconstructed semiconductor surfaces that appeared in the literature after 1990, but did not involve Si and GaAs. The years are filtered by use of the “>” relational operator (also available are “>=”, “=”, “<=”, and “<”). Several other powerful operators are available to further narrow down or expand searches for the other search criteria. These are the logical operators “OR”, “NOT”, “AND” and “BETWEEN” and the wildcard operator “*”. To exclude Si and GaAs structures, one would search with the criterion “NOT GaAs AND NOT Si”. The BETWEEN operator would set a range for the criterion. For example, the substrate criterion “BETWEEN H and S” would result in selection of just those reconstructed semiconductor structures with substrates that start in this alphabetical range of initial letters – InP, InSb etc.

3. COMPARING STRUCTURES

One of the most useful aspects of SSD-4 is the ability to display simultaneously up to three structures side by side as three-dimensional visualizations. The extensive analytical capabilities built into the visualization software, described below, allow direct comparisons of adsorption sites, bond lengths, nearest-neighbor shells and many other important items of structural interest. In compare mode, the comparison structure(s) are chosen either from a pre-selected list that results from a search, or from the full database. Figure 7 shows a comparison of two similar benzene adsorption structures, one on Pd(111) and a second on Ru(0001). The ability to see both structures at once and to be able to interrogate each one for structural data is extremely valuable.

4. THREE-DIMENSIONAL VISUALIZATION AND ANALYSIS

Another attractive feature of the new version of SSD is the immediate visualization of selected structures by 3-dimensional rectangular surface sections in a separate graphics window as shown in Fig. 4, top right panel. The view direction with respect to the surface as well as the magnification and perspective used in the figure can be changed easily by mouse dragging inside the window. In addition, the graphics window is combined with a menu bar at the top of the SSD screen, which offers various ways to manipulate the structure graphics. For example, the displayed surface section can be changed in its size and orientation to visualize further structural details. On surfaces with disordered overlayers the randomized positioning of overlayer atoms

can be varied for improved clarity. Furthermore, different graphical representations of atoms (by points, circles, or differently shaded balls) can be selected from the menu, and atoms can be connected by lines or sticks of finite thickness. In addition, the graphics menu bar includes different settings of view parameters, such as stereo or parallel/central projection views, and layout parameters, such as color assignments, framing, legends and more.

Graphics generated by the visualizer inside SSD can be saved in PostScript files to be printed on color or gray-scale PostScript printers or typesetting devices for publication-ready prints. This permits using the maximum resolution of the printing device. Furthermore, PostScript output files from SSD can be further modified for illustration purposes or for further graphical processing. As an example, Fig. 8 shows a PostScript picture of the silicon carbide (100) surface with a (2x1) reconstruction. Here four silicon atoms of the surface layer have been removed and an additional arrow points at sub-surface carbon.

The visualization of a surface structure also allows the interactive analysis of structural relationships not tabulated in the database part of SSD, such as

- distances between two atoms,
- bond angles between three atoms, angles between planes through atoms,
- neighboring shells and planes with respect to an atom,
- basis vectors visualizing the layer (and bulk) periodicity.

Such geometric quantities are “measured” by clicking on atoms of interest directly within the graphics window.

The SSD-4 surface visualizer (SURVIS) can also be used to visualize and analyze surface structures provided by ASCII files outside SSD. The corresponding input file format is explained in all details in the SSD-4 documentation. Further, the authors of SSD-4 have developed a program utility SSDIN4 which can be used by surface scientists who want to submit their own structure data for the next update of SSD. This freely distributed utility contains extensive graphical features facilitating data input and can be downloaded from the World Wide Web at <http://w3.rz-berlin.mpg.de/~hermann/ssdin4/index.html>.

ACKNOWLEDGMENTS

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REFERENCES

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- [2] P.R. Watson, M.A. Van Hove and K. Hermann, NIST Surface Structure Database - Ver. 3.0, National Institute of Standards and Technology, Gaithersburg, Maryland (1999).
- [3] M.A. Van Hove, K. Hermann, P.R. Watson and J. Rumble, in The Structure of Surfaces VI, Proc. ICSOS-VI, Eds. E. Ogryzlo, K.A.R. Mitchell and M.A. Van Hove, Surf. Rev. Lett. **6**, 805 (1999).

FIGURES

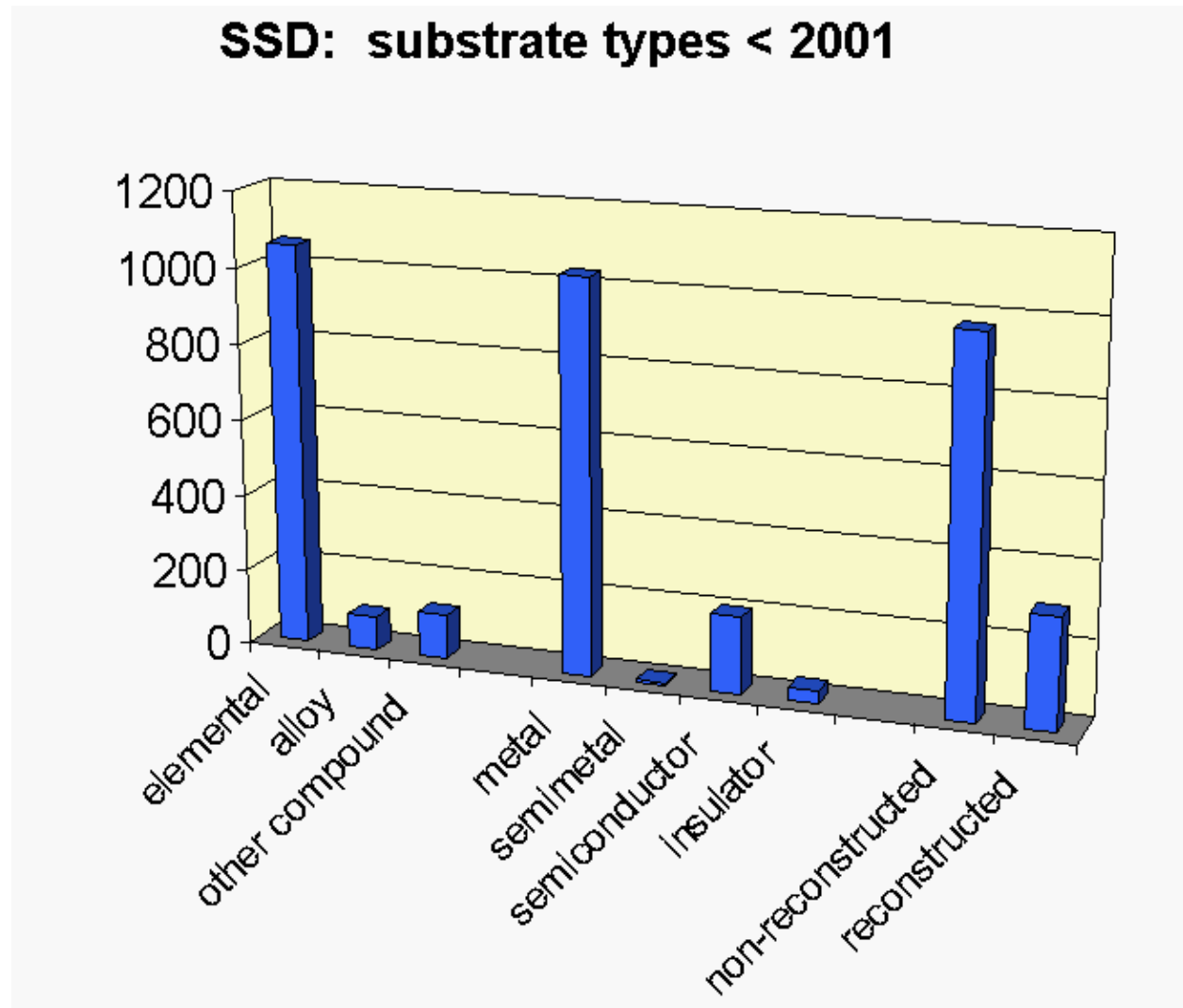


Figure 1. Histogram showing the number of structures in SSD-4 by different categories of substrate materials.

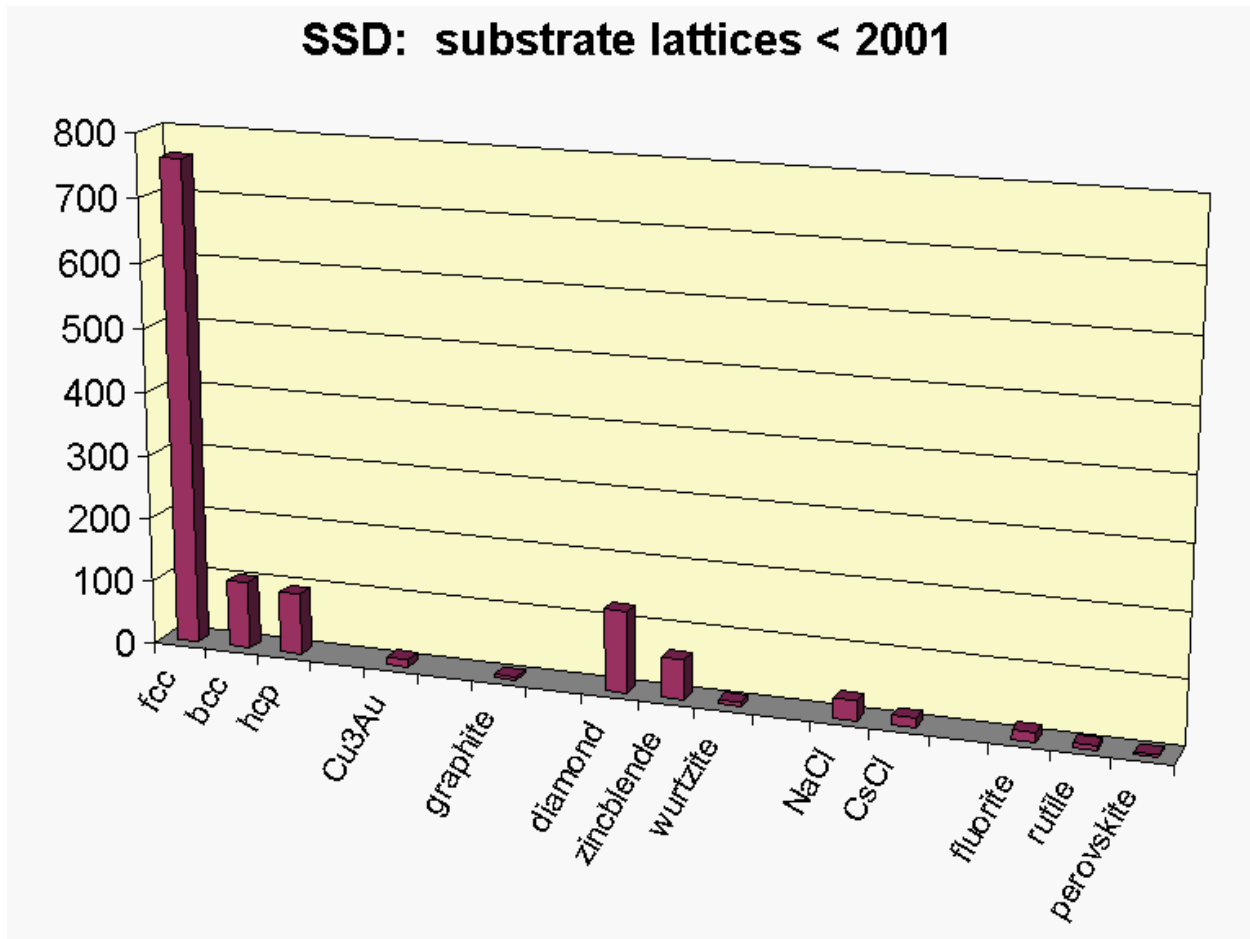


Figure 2. Histogram showing the number of structures in SSD-4 by different substrate lattices.

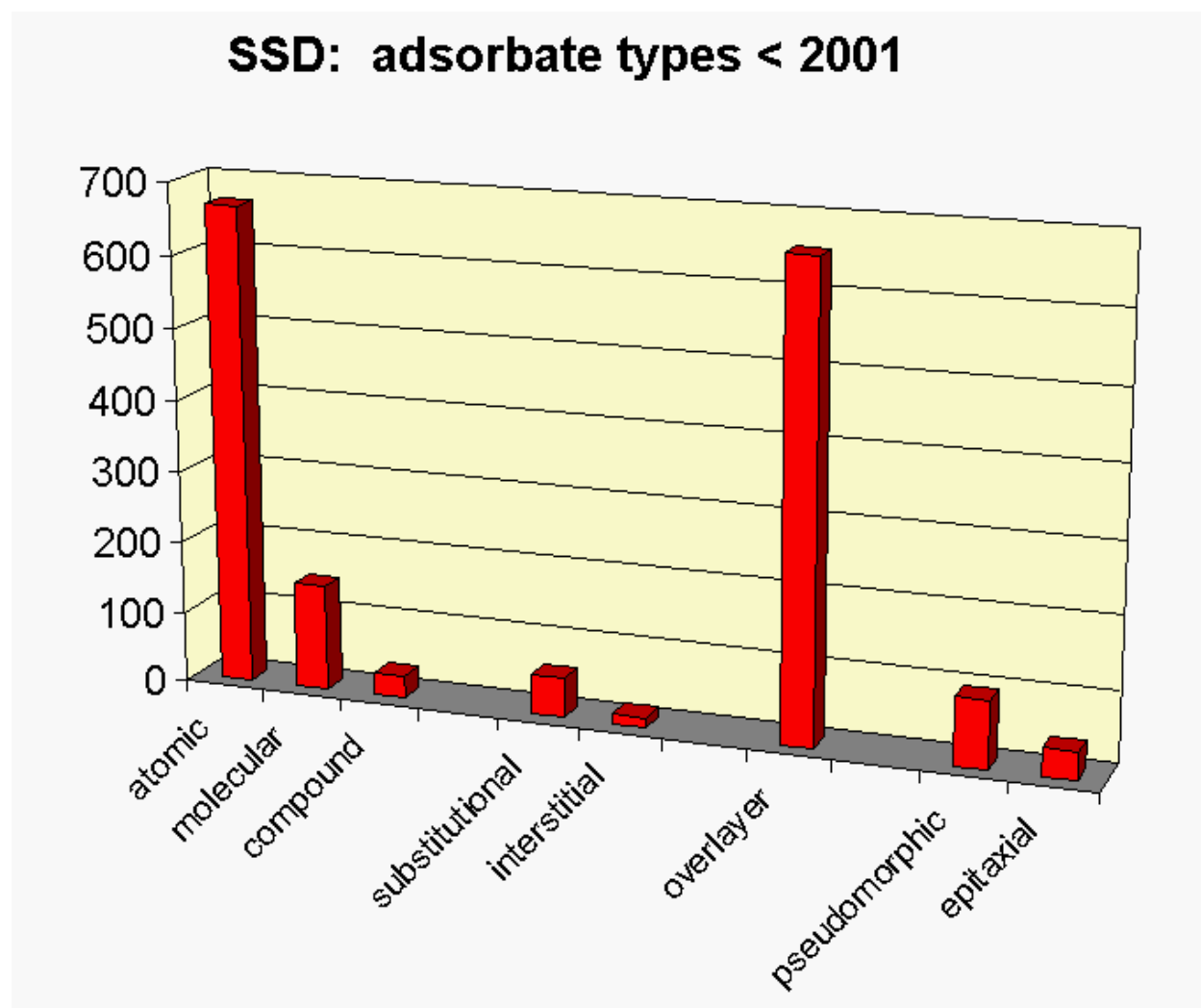


Figure 3. Histogram showing the number of structures in SSD-4 by different adsorbate types.

SSD NIST Surface Structure Database 4.0

File View Settings Analysis Re-plot Refresh Help

Experiment/Theory

Pd(111)+(3x3)-C6H6+2CO
46.6.1.8.2

Sample preparation Help Close

No. of samples: 1
Treatment: exposure to CO and benzene at room temperature
Crystallinity:
Anal. methods:
Contamination: monitored by AES and LEED

Data collection

Technique: LEED
Method:
Data set: I-V curves at normal incidence (16 beams) and off-normal incidence (29 beams); 20<E<200eV

Theory/data treatment

dynamical LEED (BSN, RFS, KSLA); 5 phase shifts; thetaD=225K

Structures examined

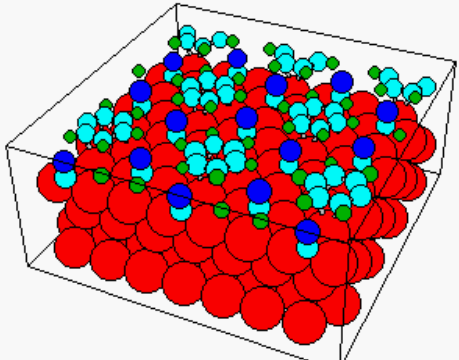
benzene in top, bridge, fcc, hcp sites with various high symmetry orientations and distortions including out of plane buckling, ring expansion and Kekule distortion; CO intact, stretched and normal to surface in same sites consistent with benzene orientations

Quality of experiment/theory fit

RVHT=0.25, RRZJ=0.49, RPE=0.48

46.6.1.8.2 : Current structure - Pd(111)+(3x3)-C6H6+2CO

Elements:
D
H
C
Pd



Structure list

Viewing 1267 out of 1267 records.

Class #	Name	Technique	Year	Authors
46.6.1.8.2	Pd(111)+(3x3)-C6H6+2CO	LEED	1988	H. Ohtani, M.A.
46.6.1.8.3	Pd(111)+(3x3)-C6H6+2CO	LEED	1994	A. Barbieri, M.A.
46.6.8.2	Pd(111)+(r3x3)R30°-CO	LEED	1987	H. Ohtani, M.A.
46.6.8.11	Pd(111)+(r3x3)R30°-CO	PED	1997	V. Fernandez, T.
46.6.8.12a	Pd(111)+c(4x2)-2CO	PED	1998	T. Giessel, O. Sci
46.6.8.13	Pd(111)+(r3x3)R30°-CO	LEED	2000	I. Zasada and M.

DATA Summary Expt/Th 2D cells Coords Bonds **MODE** Browse Search Compare **STRUCTURE** First Previous Next Last

Figure 4. Typical initial SSD-4 screen showing default windows for the Pd(111)+(3x3)-C₆H₆+2CO structure.

Experiment/Theory	
Pd(111)+(3x3)-C6H6+2CO	
46.6.1.8.2	
Sample preparation	
No. of samples	1
Treatment	exposure to CO and benzene at room temperature
Crystallinity	
Anal. methods	
Contamination	monitored by AES and LEED
Data collection	
Technique	LEED
Method	
Data set	I-V curves at normal incidence (16 beams) and off-normal incidence (29 beams); 20<E<200eV
Theory/data treatment	
dynamical LEED (BSN, RFS, KSLA); 5 phase shifts; thetaD=225K	
Structures examined	
benzene in top, bridge, fcc, hcp sites with various high symmetry orientations and distortions including out of plane buckling, ring expansion and Kekule distortion; CO intact, stretched and normal to surface in same sites consistent with benzene orientations	
Quality of experiment/theory fit	
RVHT=0.25, RRZJ=0.49, RPE=0.48	

Figure 5. SSD-4 subwindow on experiment/theory giving details about sample preparation, data collection, and more for the Rh(111)+c(2√3x4)rect-C₆H₆+CO structure.

Search criteria

Substrate: NOT GaAs AND NOT Si

- type: []

- structure: reconstructed

- elec: semiconductor

- lattice: []

- face: []

Adsorbate: []

- type: []

- structure: []

Pattern: []

Technique: []

Authors: []

Journal: []

Year of publ.: >1990

Classification #: []

Don't show Hints window again Wildcards ON

Matches found for this search: 35

Search Accept Clear Help Cancel

Figure 6. SSD-4 subwindow used for structure searches with input for finding reconstructed semiconductor structures which appeared after 1990, excluding Si and GaAs structures.

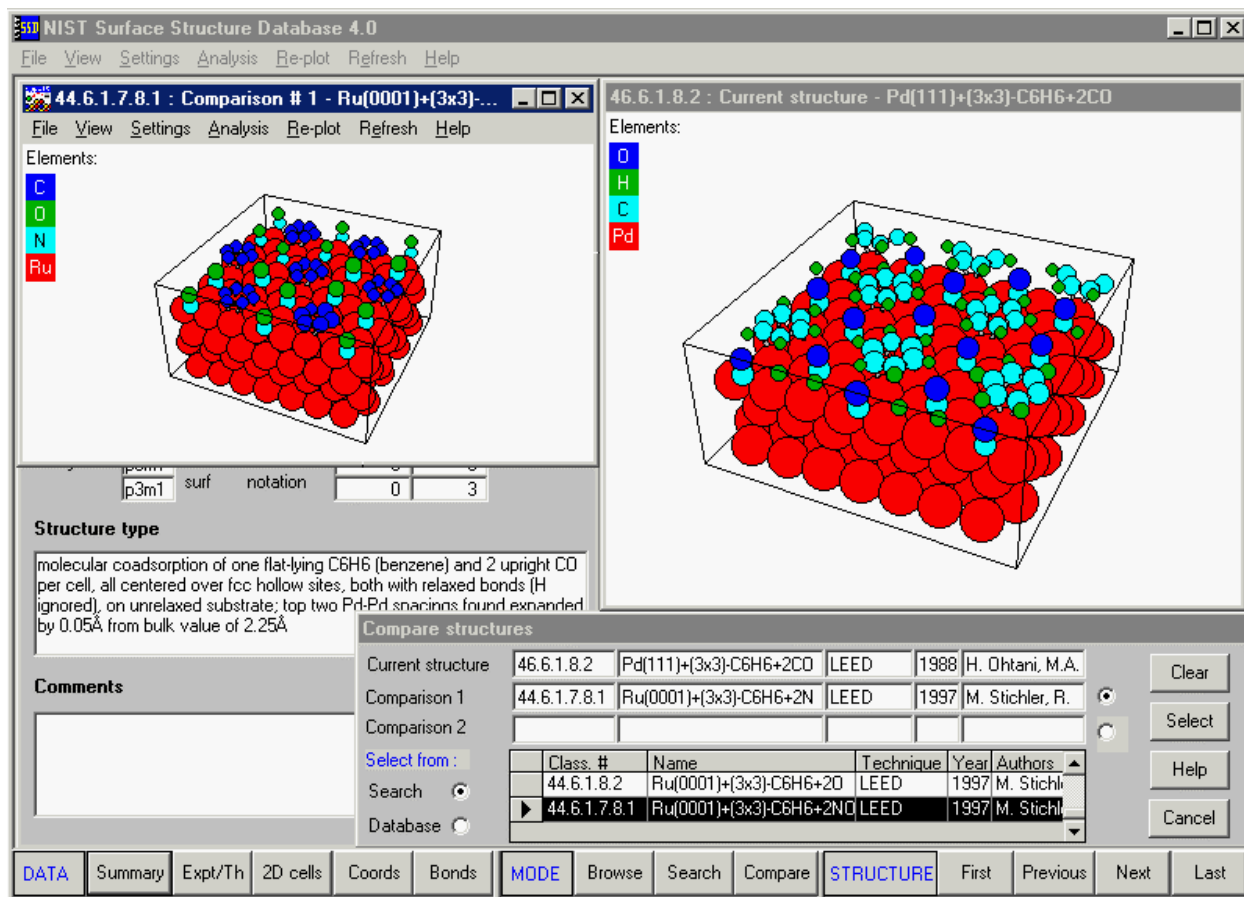
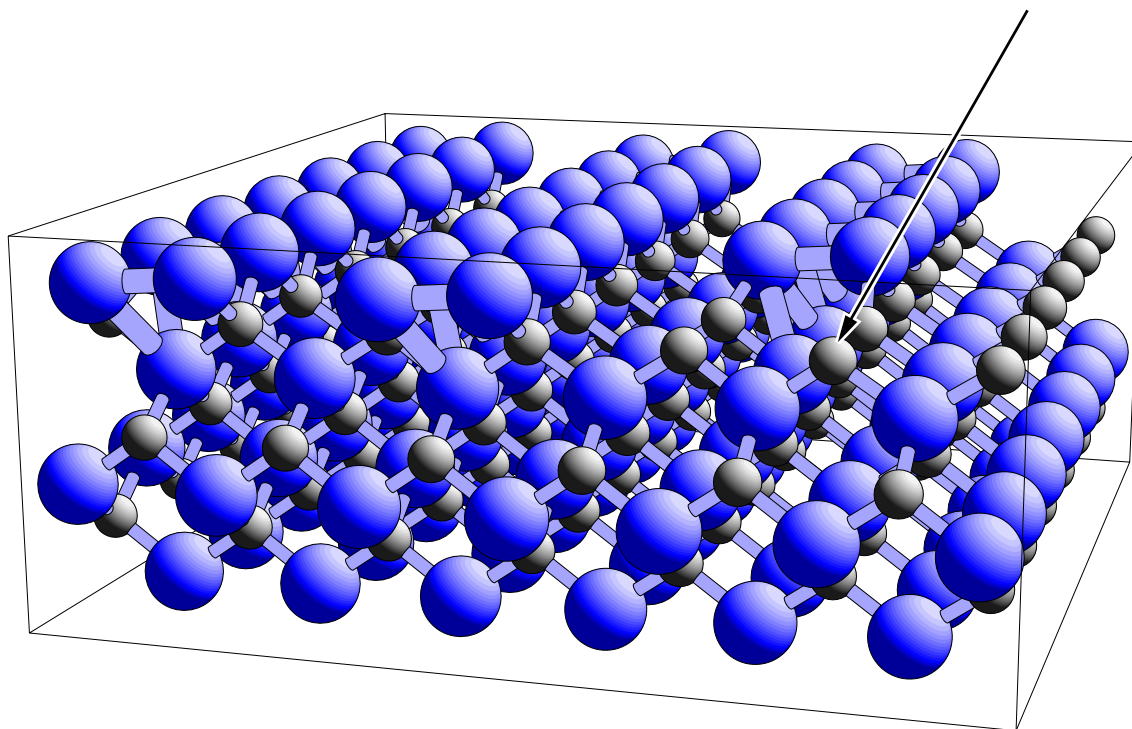


Figure 7. Comparison of two similar benzene adsorption structures on Pd(111) and on Ru(0001).



Current structure - SiC(100)-(2x1) [14.6.8]

(C) SSD/SURVIS4

Figure 8. SSD-4 PostScript print output of the silicon carbide (100) surface with a (2x1) reconstruction showing rows of Si dimers at the top. Two surface dimers (four silicon atoms) have been removed and an additional arrow points at sub-surface carbon.