

The *NIST* Surface Structure Database – SSD version 4

M. A. Van Hove,^{a*} K. Hermann^b
and P. R. Watson^c

^aMaterials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA, and Department of Physics, University of California at Davis, Davis, CA 95616, USA, ^bAbt. Theorie, Fritz-Haber Institut, Faradayweg 4-6, D-14195 Berlin, Germany, and ^cDepartment of Chemistry, Oregon State University, Corvallis, OR 97331-4003, USA

Correspondence e-mail: vanhove@lbl.gov

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SSD-4, the fourth version of the *NIST* Surface Structure Database, has appeared 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 grayscale 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:

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

The SSD includes:

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

Figs. 1–3 show the types of surface structures included in SSD-4 (Watson *et al.*, 2002). Fig. 1 counts structures by the type of substrate material, categorizing three different criteria: elemental *versus* metallic alloy *versus* other compound; metal *versus* semi-metal *versus* semiconductor *versus* insulator; and

non-reconstructed *versus* reconstructed. Fig. 2 counts structures by the lattice type of the substrate (whether clean or adsorbate-covered): f.c.c., b.c.c. *etc.* Fig. 3 counts structures by the type of adsorbate structure: atomic *versus* molecular *versus* compound adsorption; substitutional *versus* interstitial adsorption; adsorption as an overlayer; and pseudomorphic *versus* 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 (Watson *et al.*, 1999; Van Hove *et al.*, 1999).

SSD: substrate types < 2001

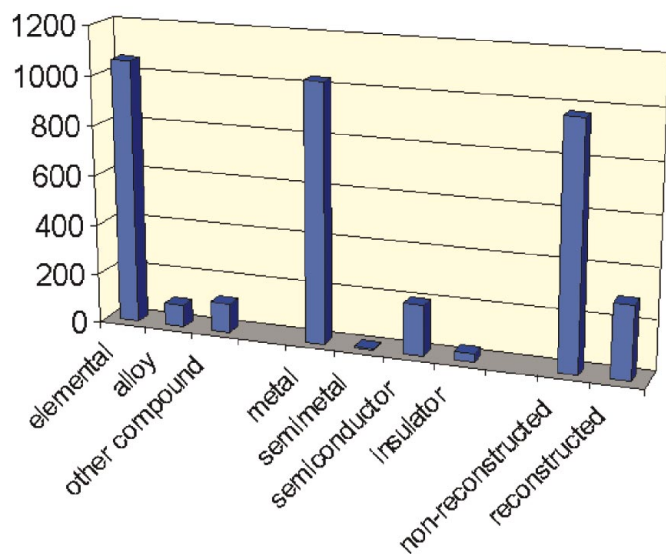


Figure 1 Histogram showing the number of structures in SSD-4 by different categories of substrate materials.

SSD: substrate lattices < 2001

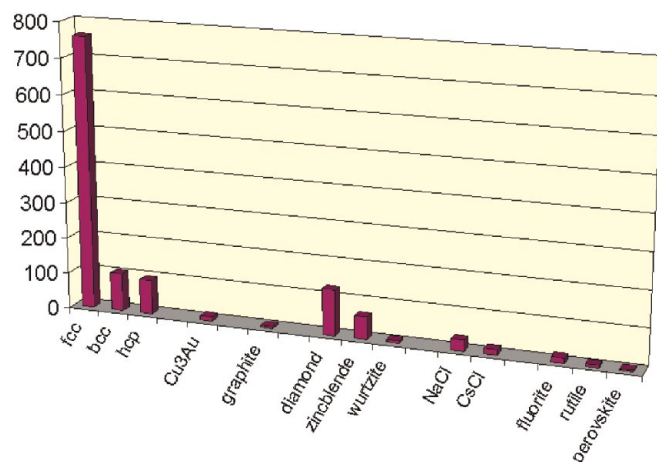


Figure 2 Histogram showing the number of structures in SSD-4 by different substrate lattices.

Fig. 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 the left and a graphics window at the right. A structure list is also shown at the bottom right, from which this particular structure was selected. At the 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 Fig. 5, which gives details about sample preparation, data collection, theory/data treatment, structures examined and the 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.

SSD: adsorbate types < 2001

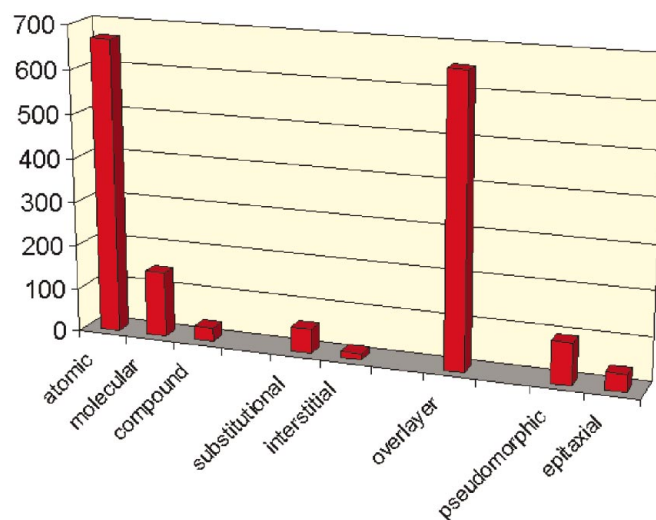


Figure 3 Histogram showing the number of structures in SSD-4 by different adsorbate types.

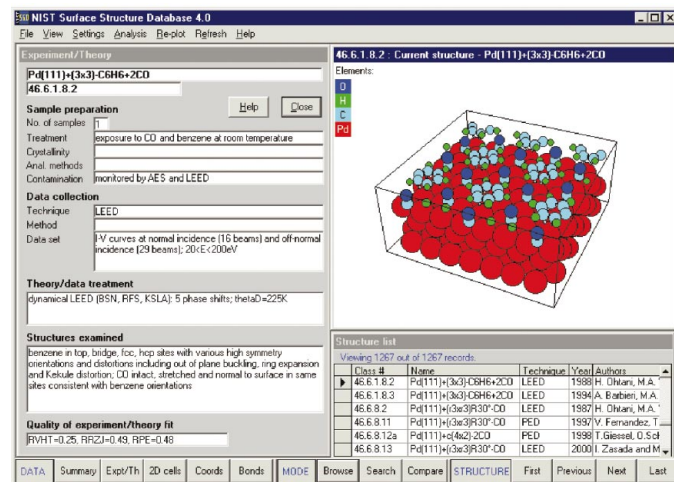


Figure 4 Typical initial SSD-4 screen showing default windows for the Pd(111) + (3 × 3) – C₆H₆ + 2CO structure.

42 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 Fig. 4. More usefully, sets of related structures can be found by searching the database. Three-dimensional pictures of up to three structures can be displayed simultaneously 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 the 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 the 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

Figure 5
SSD-4 subwindow on experiment/theory giving details about sample preparation, data collection and more for the Rh(111) + c(2(3)^{1/2} × 4)rect - C₆H₆ + CO structure.

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.

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. Fig. 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 three-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

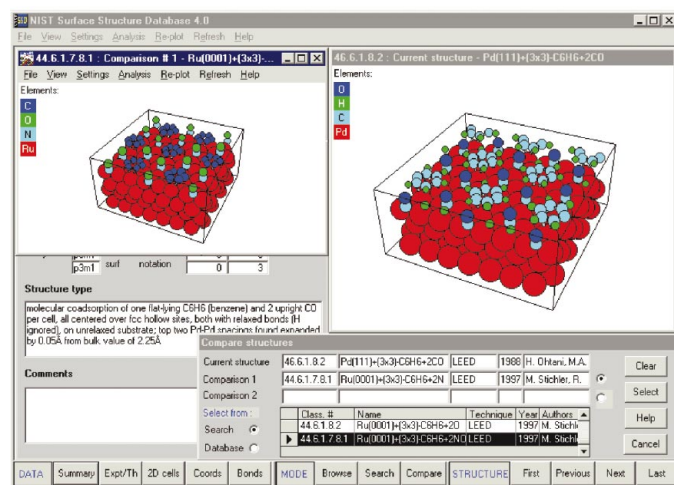


Figure 7
Comparison of two similar benzene adsorption structures on Pd(111) and on Ru(0001).

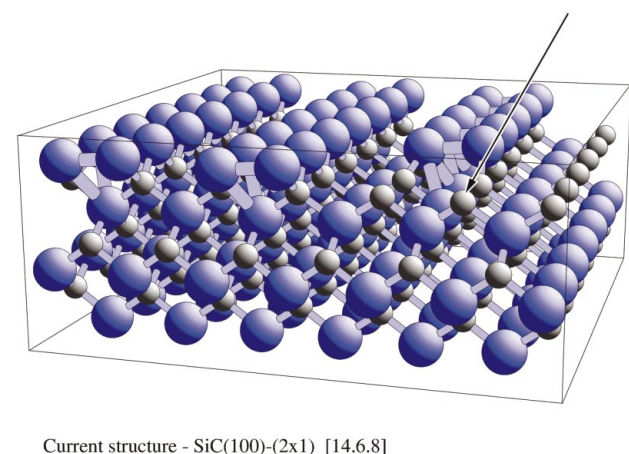


Figure 8
SSD-4 PostScript print output of the silicon carbide (100) surface with a (2 × 1) reconstruction showing rows of Si dimers at the top. Two surface dimers (four Si atoms) have been removed and an additional arrow points at subsurface carbon.

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 grayscale 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 (2 × 1) reconstruction. Here four Si atoms of the surface layer have been removed and an additional arrow points at subsurface 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:

- (i) distances between two atoms,
- (ii) bond angles between three atoms,
- (iii) angles between planes through atoms,
- (iv) neighboring shells and planes with respect to an atom,
- (v) 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 full detail 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>.

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References

Van Hove, M. A., Hermann, K., Watson, P. R. & Rumble, J. (1999). *Surf. Rev. Lett.* **6**, 805–811.

Watson, P. R., Van Hove, M. A. & Hermann, K. (1999). *NIST Surface Structure Database, Version 3.0*. National Institute of Standards and Technology, Gaithersburg, Maryland, USA.

Watson, P. R., Van Hove, M. A. & Hermann, K. (2002). *NIST Surface Structure Database, Version 4.0*. National Institute of Standards and Technology, Gaithersburg, Maryland. [Contact: Standard Reference Data Program, National Institute of Standards and Technology, Building 820, Room 113, Gaithersburg, MD 20899; <http://www.nist.gov/srd/nist42.htm>; e-mail: srdata@enh.nist.gov.]