SSD (Surface Structure Database) Data Format

The SSD format has been developed for archiving detailed surface structure data for inclusion in the NIST Surface Structure Database (SSD). This format is also used in the SSDIN program to prepare SSD input in an interactive way. All details of this format, also called **ASD** (ASCII Structure Data) format, will be described in this document. For further details consult the interactive SSDIN help file available with the SSDIN software package.

Underlined titles with bold italic font in the text refer to subsections of this document listed in the Table of Contents.

Table of Contents

SSD file format 2

General rules (SSD files) 3

Detailed data format (SSD files) 5

Examples of SSD structure files 14

Technique abbreviations 19

Journal abbreviations 22

Table of 2D Space Groups 23

Bulk / interlayer spacing 25

Region 26

Definition of 3D repeat vectors 27

Site occupancy 28

Bibliography and downloads 29

About SSDIN, SSD 30

SSD file format

This section discusses the SSD (Surface structure data) file format which is used to save the complete set of data of a given structure on ASCII type files for further processing or for submission to be included in the SSD database. **Note** that an SSD format file can contain more than one structure. The general rules for the file format are specified in subsection ***General rules (SSD files)***, the format of each data item is described in detail in subsection ***Detailed data format (SSD files)***, and example file output is shown in subsection ***Examples of SSD structure files***. For further information consult the subsections

General rules (SSD files)

Detailed data format (SSD files)

Examples of SSD structure files

General rules (SSD files)

Each structure is described by a set of numerical or textual items contained in lines of ASCII characters where the following general rules apply:

- All data items must appear in the order given by the description in subsection ***Detailed data format (SSD files)***.
- Each data item must appear either as a ‘‘free format‘‘ textual item or as a ‘‘fixed format‘‘ tabular item. Fixed format items are restricted to positions and lengths defined by the format detailed in ***Detailed data format (SSD files)***.
- No line of information may exceed 80 characters in total, including all SSD-specific special characters. Tab characters may not be used.
- A blank line in free format sections is ignored, it is not ignored in fixed format tabular data sections.
- Lines can show a command sequence at the beginning (command line, without leading blanks) where
  - ## defines the beginning of a structure in a file (mandatory for each structure),
  - #ff defines the end of a structure in a file (mandatory for each structure) ,
  - #c defines a comment line (free format text or numbers) which is ignored upon input. **Note** that comment lines are NOT allowed in fixed format tabular data sections,
  - #tx where x = a, b, c, d, e or f, starts a fixed format tabular data section,
  - #fx where x = a, b, c, d, e or f, finishes a fixed format tabular data section.

  Note that all information following the above command sequence on the same line is ignored upon input. New data must start on a subsequent line. Command lines #tx and #fx must both enclose a fixed format tabular data section.
- Lines without a command sequence can contain either one free format item, or only fixed format items. No mixing of free and fixed format items is allowed on the same line.
- Tabular data of fixed format must fit within a specific range of columns, as described in ***Detailed data format (SSD files)***, where ‘‘An‘‘ refers textual ASCII data (e. g. ‘‘`p3m1`‘‘ is of A4 format), ‘‘Nn‘‘ denotes numerical data (real or integer valued, e. g. ‘‘`3.0000`‘‘ is of N6 format, ‘‘ `-14`‘‘ is of N4 format).
- Each structure MUST contain each of the six tabular data sections (#ta-#fa through #tf-#ff) and sections must appear in the alphabetic sequence (i. e. a – f).
- Numerical data of fixed format (real or integer) cannot use exponential representation (e. g. 1.5E3). The number of digits after the decimal point of a real quantity is limited only by the allowed length of the format field. The decimal point may be positioned freely within the allowed format field.
- Leading and trailing blanks in alphanumeric fields are ignored upon input.
- A blank numerical field is interpreted as a zero number while a blank alphanumeric field is ignored.
- Free format textual items are given in the form (the enclosing double quotes MUST appear on the line and only one item per line is allowed)
  - ‘‘sn:STRING’‘, n = 1 to 17, 22 to 37, (outline section),
  - ‘‘tn:STRING’‘, n = 1 to 16, (technique section),
  - ‘‘2dn:STRING‘‘, n = 8, 14, (2D parameter section),
  - ‘‘3dn:STRING‘‘, n = 1 to 4, (3D parameter section),
  - ‘‘bn:STRING‘‘, n = 1, 7, (Bond distances / angles section),

  where STRING denotes an ASCII string with textual information. **Note** that special characters (see below) and double quotes (‘‘) must not appear in ASCII strings STRING. Strings may have any length up to the limit given with the string definition in (B).

- Free format textual items can be omitted if necessary. Items of the same type (s, t, 2d, 3d, b) must appear in correct numerical order (e. g. item ‘‘s6:…’‘ must appear after item ‘‘s4:…’‘).
- Free format textual items may contain special characters which must be ASCII coded using the table below. Special characters must NOT be entered by their PC keyboard code (3 digits keeping the **ALT** key pressed). Powers of 10 should be denoted as, for example: 1.5E-10 in textual items. The following special characters should be represented either by the corresponding fully-spelled-out 6-character sequence Altnnn, or preferably by the 2-character symbol of type \x (the latter requires less space):

≈	Alt247	\=
∝	Alt224	\a (i.e. same as α)
±	Alt241	\+
∝	Alt236	\i
²	Alt253	\2 (square)
√	Alt251	\R
°	Alt248	\0 (degree, 0 = zero)
Å	Alt143	\A
α	Alt224	\a (lower case alpha)
β	Alt225	\b (lower case beta)
Γ	Alt226	\G (upper case gamma)
δ	Alt235	\d (lower case delta)
ε	Alt238	\e (lower case epsilon)
η	Alt252	\E (lower case eta)
ϕ	Alt237	\f (lower case phi)
Φ	Alt232	\F (upper case phi)
μ	Alt230	\m (lower case mu)
Π	Alt227	\P (upper case pi, upper case character not available: use \p)
σ	Alt229	\s (lower case sigma)
Σ	Alt228	\S (upper case sigma)
τ	Alt231	\T (lower case tau)
θ	Alt233	\t (upper case theta)
Ω	Alt234	\O (upper case omega, O = upper case letter O)

- The minimum file content for a meaningful structure is:

  ##
  item ‘‘s1:structure name’‘
  data blocks #ta-#fa, #tf-#fb
  item [2d8]
  data block #tc-#fc
  item [2d14]
  data blocks (#td-#fd through #tf-#ff)

Detailed data format (SSD files)

In the following the formats of all data item are described in detail. Each item is defined by a length (of n characters) where **An** refers textual ASCII data (e. g. ‘‘p3m1’‘ is of A4 format), **Nn** denotes numerical data (real or integer valued, e. g. ‘‘3.0000’‘ is of N6 format, ‘‘ -14’‘ is of N4 format). **Note** that the sequence of items MUST be given in the order given below.

Note that all **textual lines** (i. e. lines 1-17, 21-38, 43, 47, 51, 60) MUST be enclosed by **double quotes**. The format specifications given below for textual lines do not include the mandatory double quotes, see also ***Examples of SSD structure files***.

(a) Beginning and Outline section

Line 0 **(‘## Beginning of structure’)**

Starting command line of structure description

Line(s) 1 **(‘s1:’, A60, / ‘s1:’, A60)** **TITLE(1), TITLE(2)**

Common name of the structure. Up to 120 characters are allowed where the two strings, TITLE(1), TITLE(2), are combined to one title (without a separating space for a continuous title).
Example: ‘‘s1: Al(111)+(\R3x\R3)R30\0-Li’‘.

Line 2 **(‘s2:’, A20)** **CLASS**

Class number of the structure giving a shorthand notation. Parameter CLASS is used only for internal purposes and needs not to be provided by the user.
Example: ‘‘s2:13.3.1’‘

Line 3 **(‘s3:’, A40)** **STATUS**

Status of the structure wrt. SSD processing. Parameter STATUS is used only for internal purposes and needs not to be provided by the user.
Example: ‘‘s3:new in SSD3’‘

Line 4 **(‘s4:’, A20)** **TECHNIQUE**

Experimental technique used to determine the structure. Abbreviations of possible techniques are given in section ***Technique abbreviations***.
Example: ‘‘s4:LEED’‘.

Line(s) 5 **(‘s5:’, A60 / ‘s5:’, A60)** **AUTHORS(1), AUTHORS(2)**

List of authors. Up to 120 characters are allowed where the two strings, AUTHORS(1), AUTHORS(2), are combined to one author list (with a separating space to separate between authors). If more authors exist than will fit in 120 characters, they may be inserted in the comments items [s28-s32]. **Note** that authors' names may not include accents of any kind. Further, the umlaut vowel (double dotted vowel) in German, Finnish or other names should be replaced by the vowel plus an extra letter ‘‘e’‘ yielding, e. g. ‘‘Mueller’‘, ‘‘Haekinnen’‘ etc.
Example: ‘‘s5:M.M. Nielsen, S.V. Christensen and D.L. Adams’‘

Line 6 **(‘s6:’, A40)** **JOURNAL**

Name of journal where the structure has been published. Names of most frequently cited journals are given in section ***Journal abbreviations***.

Example: ‘‘s6:Phys. Rev.‘‘

Line 7 (‘s7:’, A8) VOLUME

Volume number of journal where the structure has been published. .
Example: ‘‘s7:B54‘‘

Line 8 (‘s8:’, A8) PAGE

Page number of journal issue where the structure has been published. .
Example: ‘‘s8:17902‘‘

Line 9 (‘s9:’, N10) YEAR

Year of journal issue where the structure has been published. .
Example: ‘‘s9:1996‘‘

Line 10 (‘s10:’, A20) SUBSTRATE

Full name of the substrate included in the structure.
Example: ‘‘s10:Al‘‘

Line 11 (‘s11:’, A20) BULK_LATTICE

Crystallographic name of the lattice describing the substrate. Here short Bravais lattice names are preferred (e. g. ‘‘fcc‘‘ rather than ‘‘face centered cubic’‘).
Example: ‘‘s11:fcc‘‘

Line 12 (‘s12:’, A20) CRYSTAL_FACE

Lattice direction of the crystal face (net plane direction) describing the substrate surface. Directions are described by Miller indices using both 3- and 4-index notation (the latter for hexagonal crystal faces) where indices are not separated by blank spaces but by commas (if needed) and are enclosed by parentheses.
Example: ‘‘s12:(111)‘‘

Line 13 (‘s13:’, A4) SUBSTRATE_SYMMETRY

2-dimensional symmetry group describing the symmetry of the 2-dimensional substate unit cell. Any of the 21 (17 plus 4, see ***Table of 2D Space Groups***) space group labels may be used where possible labels are listed in the ‘‘type‘‘ column of the space group table of section ***Table of 2D Space Groups***. **Note** that only the short notation is accepted (e. g. ‘‘pmm‘‘ rather than ‘‘p2mm’‘).
Example: ‘‘s13:p3m1‘‘

Line 14 (‘s14:’, A4) SURFACE_SYMMETRY

2-dimensional symmetry group describing the symmetry of the complete surface including substrate and all superlattice cells. Any of the 21 (17 plus 4, see ***Table of 2D Space Groups***) space group labels may be used where possible labels are listed in the ‘‘type‘‘ column of the space group table of section ***Table of 2D Space Groups***. **Note** that only the short notation is accepted (e. g. ‘‘pmm‘‘ rather than ‘‘p2mm’‘).
Example: ‘‘s14:p31m‘‘

Line(s) 15 (‘s15:’, A60 / ‘s15:’, A60) ADSORBATE(1), ADSORBATE (2)

Adsorbate definition in two parts given on two lines where ADSORBATE(1) contains adsorbate formula(s) and ADSORBATE(2) gives common molecular name(s). A semicolon ‘‘;‘‘ is used to separate coadsorbates within the lines (e. g. ‘‘s15:CO;C6H6‘‘, followed on the next line by ‘‘s15:carbon monoxide; benzene‘‘). The second line of the adsorbate definition is optional.

Example: ‘‘s15:Li‘‘ / ‘‘s15:Lithium‘‘.

Line 16 (‘s16:’, A20) COVERAGE

Adsorbate coverage. The coverage may be given in numerical or verbal form and should include the reference unit cell.
Example: ‘‘s16:1/3 Li/Al‘‘

Line 17 (‘s17:’, A20) PATTERN

Common name of the surface periodicity wrt. to the substrate lattice. Here both Wood notation (e. g. ‘‘c(2x2)‘‘) and (2x2) matrix definitions (e. g. ‘‘(1,-1|1,1)‘‘) are allowed.
Example: ‘‘s17:(\R3x\R3)R30\0‘‘ for a (√3x√3)R30° superlattice structure

Line 18 (‘#ta’) start of tabular section a

Line 19 (N10, N10, N10, N10) M11, M12, M21, M22

2x2 Matrix defining the 2-dimensional periodicity of the complete surface including substrate and all superlattice cells where the substrate lattice is used as a reference.
Note that the matrix can contain non-integer valued components in cases of incommensurate superlattices.
Example: ‘‘ 1.0000 1.0000 -2.0000 1.0000‘‘

Line 20 (‘#fa’) end of tabular section a

Line 21 (‘s22:’, A5) TEMPERATURE

Temperature at which the structure was determined. The temperature value should be combined with a unit (C = Celsius, F = Fahrenheit, K = Kelvin). Abbreviations (e. g. ‘‘RT‘‘ for room temperature) should be avoided.
Example: ‘‘s22:100K‘‘

Line(s) 22 (‘s23:’, A60 / ‘s24:’, A60 / ‘s25:’, A60 /‘s26:’, A60 /‘s27:’, A60)
STRUCTURE_TYPE(1 – 5)

Verbal description of the complete structure (in up to five lines) emphasizing all characteristic features, so that the structure can be understood without looking at the coordinates or a graph. This information could, for instance, state whether a surface is relaxed (and, if so, to what depth) or reconstructed (and, if so, in what fashion), whether the surface has an overlayer or buried underlayer, which adsorption sites are occupied, etc.
Example: ‘‘s23:adatoms in substitutional sites in top Al layer‘‘

Line(s) 23 (‘s28:’, A60 / ‘s29:’, A60 / ‘s30:’, A60 /‘s31:’, A60 /‘s32:’, A60)
COMMENTS(1 – 5)

These (up to five) line(s) can contain any useful remarks that don't fit elsewhere, e.g., additional authors, special temperature- or coverage-dependent behavior, a reference to a related structure, etc.
Example: ‘‘s28:prior to LEED measurements, surface was flashed to‘‘,
‘‘s29:850K to eliminate H (which desorbs at 360K)‘‘

Line 24 (‘s33:’, A60) SUBSTRATE_TYPE

This line defines the substrate as ‘‘elemental‘‘, ‘‘compound‘‘ or ‘‘alloy‘‘ type. Different keyword are separated by semicolons (;).
Example: ‘‘s33:elemental‘‘

Line 25 (‘s34:’, A60) ELECTRONIC_STATE

This line defines the electronic state of the substrate as ‘‘metal’‘, ‘‘semimetal’‘, ‘‘semiconductor’‘, ‘‘insulator’‘, or ‘‘other’‘ type. Different keyword are separated by semicolons (;).
Example: ‘‘s34:metal’‘

Line 26 (‘s35:’, A60) SUBSTRATE_RECONSTRUCTION

This line defines the reconstruction state of the substrate as ‘‘reconstructed’‘ or ‘‘non-reconstructed’‘.
Example: ‘‘s35:reconstructed’‘

Line 27 (‘s36:’, A60) ADSORBATE_TYPE

This line defines the adsorbate type as ‘‘atomic’‘, ‘‘molecular’‘, ‘‘film’‘, ‘‘compound’‘, or a combination thereof. Different keyword are separated by semicolons (;).
Example: ‘‘s36:atomic’‘

Line 28 (‘s37:’, A60) ADSORBATE_STRUCTURE

This line qualifies the adsorbate structure as’‘overlayer’‘, ‘‘interstitial’‘, ‘‘substitutional’‘, ‘‘epitaxial’‘, ‘‘pseudomorphic’‘ or a combination thereof. Different keyword are separated by semicolons (;). **Note** that pseudomorphic is a particular case of epitaxial, when the 2D lattices of the film and substrate are commensurate. Use ‘‘epitaxial’‘ only for incommensurate cases.
Example: ‘‘s37:substitutional’‘

(b) Technique section

Line 29 (‘t1:’, A2) SAMPLES

Number of samples used to check the experimental reproducibility.
Example: ‘‘t1:1’‘

Line 30 (‘t2:’, A60) TREATMENT

This describes the substrate preparation and/or the adsorption method.
Example: ‘‘t2:Li deposited at 300K’‘

Line 31 (‘t3:’, A40) CRYSTALLINITY

This describes any indication of the degree of crystalline perfection (e.g., sharp LEED spots).
Example: ‘‘t3:LEED: sharp spots, low background’‘

Line 32 (‘t4:’, A60) ANALYSIS_METHODS

This describes any methods other than the primary structure determination technique (e. g. AES and/or XPS) used to evaluate the preparation, perfection, coverage, adsorbate state, contamination level, etc.
Example: ‘‘t4:AES, XPS, TPD’‘

Line 33 (‘t5:’, A40) CONTAMINATION

This characterizes the level of contamination by impurities (e.g., Auger estimates).
Example: ‘‘t5:AES: C < 0.03ML’‘

Line 34 (‘t6:’, A40) DATA_COLLECTION

This describes the main measurement technique used to collect the data.

Example: ‘‘t6:video LEED’‘

Line(s) 35 (‘t7:’, A60 / ‘t8:’, A60) DATASETS(1), DATASETS(2)

This gives the nature of the experimental database (e.g., I-V curves in LEED) and a measure of its size (e.g., number of beams in LEED). Up to 120 characters are allowed where the two strings, DATASETS(1), DATASETS(2), are combined to one line of information (with a separating space).
Example: ‘‘t7:IV spectra for 14/29 symm.-ineq. beams at \t=0/15\0;’‘,
‘‘t8:E range 40-400eV’‘

Line(s) 36 (‘t9:’, A60 / ‘t10:’, A60) THEORY(1), THEORY(2)

This describes the method of the data treatment (averaging, smoothing, etc.) and of the theoretical analysis (dynamical/tensor LEED, etc.). Up to 120 characters are allowed where the two strings, THEORY(1), THEORY(2), are combined to one line of information (with a separating space).
Example: ‘‘t9:dynamical LEED (layer doubling): 14 ph shs from Moruzzi et’‘,
‘‘t10:al pots; rms vibs fitted for Li, Al in 1st, 2nd, bulk layers’‘

Line(s) 37 (‘t11:’, A60 / ‘t12:’, A60 / ‘t13:’, A60 /‘t14:’, A60 /‘t15:’, A60)
STRUCTURES_EXAMINED(1 – 5)

Verbal description (in up to five lines) of the structures which have been tested in the analysis. This may specify which structures can be excluded based on this study.
Example: ‘‘t11:adsorption in fcc hollow, hcp hollow, top and substitutional’‘,
‘‘t12:in-top-layer sites; for substitutional site, fitting of top’‘,
‘‘t13:4 interlayer spacings, and lateral position of 2nd Al layer’‘

Line 38 (‘t16:’, A40) DATA_FIT

This describes the quality of the experiment/theory fit by a qualitative or quantitative measure, such as R-factor values.
Example: ‘‘t16:chi^2=0.033’‘

(c) 2-dimensional parameter section

Line 39 (‘#tb’) start of tabular section b

Line 40 (N10, N10, N10, N10, N10) AX, AY, BX, BY, PHI

Cartesian components of the two 2-dim. lattice vectors (AX, AY) and (BX, BY) describing the substrate periodicity. PHI denotes the angle between the vectors.
Example: ‘‘2.8525 .0000 1.4262 2.4703 60.0005’‘

Line 41 (N4, N4) NDOMAIN, NSCELLS

NDOMAIN gives the number of different domain orientations are allowed (and normally observed).
NSCELLS gives the number of different superlattice cells determining the complete structure. Up to 4 different supercells are allowed (cases with more than one supercell are very rare).
Example: ‘‘ 1 1’‘

Line 42 (‘#fb’) end of tabular section b

Lines 43 – 50 are repeated for each supercell definition, i. e. NSCELLS times

(k = 1 … NSCELLS)

Line 43 **(‘2d8:’, A40)** **SUPERCELL_TYPE(k)**

This describes the type of supercell i where keywords **‘‘sk’‘** (commensurate superlattice), **‘‘ik’‘** (incommensurate lattice), **‘‘ndk’‘** (non-reconstructive lattice-gas disorder), **‘‘rdk’‘** (reconstructive lattice-gas disorder), **‘‘mk’‘** (randomly mixed layer), **‘‘b’‘** (bulk-like (1x1) lattice) are available k = 1, 2, 3 or 4.
Example: ‘‘2d8:s1’‘

Line 44 **(‘#tc’)** start of tabular section c

Line 45 **(N10, N10, N10, N10, N10)** **AsX(k), AsY(k), BsX(k), BsY(k), PHIs(k)**

Cartesian components of the two 2-dim. lattice vectors (AsX, AsY) and (BsX, BsY) describing the periodicity of supercell k. PHIs denotes the angle between the vectors.
Example: ‘‘4.2787 2.4703 -4.2788 2.4703 120.0008’‘

Line 46 **(‘#fc’)** end of tabular section c

Line 47 **(‘2d14:’, A20)** **SUPERCELL_PATTERN(k)**

This describes the LEED pattern of a structure. Here both Wood notation (e. g. ‘‘c(2x2)’‘) and (2x2) matrix definitions (e. g. ‘‘(1,-1|1,1)’‘) are allowed.
Example: ‘‘2d14:(\R3x\R3)R30\0’‘ for a (√3x√3)R30° superlattice

Line 48 **(‘#td’)** start of tabular section d

Line 49 **(N10, N10, N10, N10, A5)** **M11(k), M12(k), M21(k), M22(k), SYMM(k)**

2x2 Matrix defining the 2-dimensional periodicity of supercell k where the substrate lattice is used as a reference. **Note** that the matrix can contain non-integer valued components in cases of incommensurate superlattices. SYMM denotes the symmetry group describing the 2D symmetry of the supercell. Any of the 21 (17 plus 4, see ***Table of 2D Space Groups***) space group labels may be used (short notation only).
Example: ‘‘ 1.0000 1.0000 -2.0000 1.0000 p31m’‘

Line 50 **(‘#fd’)** end of tabular section d

(d) 3-dimensional parameter section

Line(s) 51 **(‘3d1:’, A60 / ‘3d2:’, A60 / ‘3d3:’, A60 /‘3d4:’, A60)**
ATOM_RELATIONS(1 – 4)

Verbal description (in up to five lines) of the atomic relationships making it clear which atoms form which characteristic features of the structure.
Example: ‘‘3d1:Li1: adatom in substitutional site;’‘
‘‘3d2:Al2-3: remaining Al atoms of top Al layer’‘

Line 52 **(‘#te’)** start of tabular section e

Line 53 **(N10)** **ZBULK**

ZBULK defines the bulk substrate interlayer spacing (which is also used as a reference for relative spacing differences in %). This spacing equals, in most cases, the bulk layer-to-layer repeat distance. For exceptions, see ***Bulk / interlayer spacing***.
Example: ‘‘ 2.3291’‘

Line 54 (N4) NATOT

NATOT defines the number of inequivalent atoms included in the structure.
Example: ‘‘ 7‘‘

Line 55 (A26, N10, A1, N10, A1, N10) DUMMY, XAT, UNIT, YAT, UNIT, ZAT

Definition of interlayer translation vector describing the periodicity of the **epilayer** stacking. The vector is given by (XAT, YAT, ZAT) where XAT, YAT are components parallel and ZAT normal to the surface. (**Note** that ZAT < 0 or zero for epilayers). ZAT is always defined in Angstrom. If the unit label UNIT reads ‘‘A‘‘, XAT and YAT are defined in Angstrom whereas for UNIT = ‘‘f‘‘, XAT and YAT are defined in relative units (as linear combinations of the epilayer cell vectors).
DUMMY = (‘‘epir -2‘‘ + 14 blanks) serves only as a position locator in the line.
Example: ‘‘epir -2 .0000A .0000A .0000‘‘

Line 56 (A26, N10, A1, N10, A1, N10) DUMMY, XAT, UNIT, YAT, UNIT, ZAT

Definition of interlayer translation vector describing the periodicity of the **substrate** layer stacking. The vector is given by (XAT, YAT, ZAT) where XAT, YAT are components parallel and ZAT normal to the surface. (**Note** that ZAT > 0 or zero for substrate layers). ZAT is always defined in Angstrom. If the unit label UNIT reads ‘‘A‘‘, XAT and YAT are defined in Angstrom whereas for UNIT = ‘‘f‘‘, XAT and YAT are defined in relative units (as linear combinations of the epilayer cell vectors).
DUMMY = (‘‘subr -1‘‘ + 14 blanks) serves only as a position locator in the line.
Example: ‘‘subr -1 .0000A 1.6470A 2.3291‘‘

Lines 57, (57a,) 58 are repeated for each atom, i. e. NATOT times (k = 1 … NATOT)

Line 57 (A4, A3, N5, A4, N6, N4, N10, A1, N10, A1, N10, N10, A2)
REGN, EL, NAT, CTYP, OCC, REL, XAT, UNIT, YAT, UNIT, ZAT, ZREL, SHIFT

Definition of all parameters relating to atom k of the structure.
REGN defines the region of atom k where keywords **‘‘ovrl’‘, ‘‘intf’‘, ‘‘subl’‘, ‘‘epil’‘** are available, see ***Region***.
EL defines the element name of atom k where standard names (‘‘H‘‘, ‘‘Cu‘‘, …) including ‘‘Du‘‘ for dummy atoms are used.
NAT is the number of atom k in the list (NAT = k).
CTYP defines the cell type of atom k where keywords are taken from the cell definition(s) in line(s) 43.
OCC defines the site occupancy of atom k, see ***Site occupancy***.
REL defines a number of a reference atom wrt. which the position of atom k is defined in the following . Referencing is possible only wrt. atoms which have been defined before. REL = 0 specifies absolute coordinates (i. e. no referencing) and has to be used for the first atom in the list.
Vector **(XAT, YAT, ZAT)** defines the position of atom k where XAT, YAT are components parallel and ZAT normal to the surface. ZAT is always defined in Angstrom. If the unit label **UNIT** reads **‘‘A’‘**, XAT and YAT are defined in Angstrom whereas for UNIT = **‘‘f’‘**, XAT and YAT are defined in relative units (as linear combinations of the corresponding cell vectors).
ZREL defines the relative z position (in percent) of atom k, i. e.
ZREL = ZAT/ZATbulk where ZATbulk is the z component of the substrate vector defined in line 57.
If **SHIFT = ‘‘ SH’‘** then the final atom position vf = (XAT, YAT, ZAT) is decomposed into an initial position vi = (x, y, z) and a position shift vector sh = (shx, shy, shz) (i. e. vf = vi + sh) where the shift vector is defined on the following (optional) line. Else vf defines the initial and the final atom position. Shifting may be useful to facilitate the

definition of complicated atom positions.
Example: ‘‘intf Al 2 s1 .333 1 .6667f .3333f .4100 17.6034’‘

LINE 57a (A26, N10, A1, N10, A1, N10) DUMMY, SHX, UNIT, SHY, UNIT, SHZ

This line appears only if SHIFT = ‘‘SH’‘ on the previous line 58.
Vector **(SHX, SHY, SHZ)** defines the (optional) position shift vector of atom k where SHX, SHY are components parallel and SHZ normal to the surface. SHZ is always defined in Angstrom. If unit label **UNIT** reads **‘‘A’‘**, SHX and SHY are defined in Angstrom, for UNIT = **‘‘f’‘**, SHX and SHY are defined in relative units (as linear combinations of the corresponding cell vectors). For UNIT = **‘‘c’‘**, SHX and SHY are defined in polar coordinates (i. e. SHX = distance wrt. initial position, SHY = polar angle, where SHY = 0 for the direction parallel to the first cell vector ((Ax, Ay) or (Asx, Asy)) of the corresponding substrate or supercell).
DUMMY consists of 26 blank characters.
Example: ‘‘ .1000f .1000f .0000’‘

Line 58 (A26, N10, A1, N10, A1, N10) DUMMY, XERR, UNIT, YERR, UNIT, ZERR, RZERR

DUMMY consists of 26 blank characters.
Vector **(XERR, YERR, ZERR)** combines the experimentally determined error bars on the coordinates of atom k, in the same units (Å or f) as the corresponding coordinates (labels **UNIT** of lines 57 and 58 must agree). Error bars need to be given only for coordinates that were fit to experiment. A blank entry or zero value must be given if the corresponding coordinate value was assumed rather than fit.
RZERR defines the relative z error bar (in percent) of atom k, i. e.
RZERR = ZERR/ZATbulk where ZATbulk is the z component of the substrate vector defined in line 57.
Example: ‘‘ .0100f .0100f .0200 5.000’‘

Line 59 (‘#fe’) end of tabular section e

(e) Bond distances / angles section

Line 60 (‘b1:’, A60) DISTANGLES_COMMENT

Depending on the structure determination technique, bond distances and angles can be derived from the best-fit coordinates, or vice versa, namely the coordinates can be derived from best-fit bond distances and angles. This comment line specifies which way it is and may contain any other useful comments about bond distances and angles.
Example: ‘‘b1:bond distances and angles are derived from coordinates’‘

Line 61 (‘#tf’) start of tabular section f

Line 62 (N4) NBONDS

NBONDS defines the number of bond distance / angle lines to be given on the following.
Example: ‘‘ 4’‘

Line 63 is repeated for each bond distance / angle line, i. e. NBONDS times (k = 1 … NBONDS)

Line 63 (N10, A12, A12, A12, N10) DIST12, ATOM1, ATOM2, ATOM3, ANGLE123

ATOM1, ATOM2, ATOM3 are names of three different atoms while **DIST12** defines the distance between atom 1 and 2 and **ANGLE123** defines the angle of the connection 1

– 2 –3.
Example: ‘‘ 2.8819 Li1 Al2 Al3 60.3315’‘

Line 64 (‘#ff’) end of tabular section f

This finishes the complete structure input.

Examples of SSD structure files

In the following we give three examples of SSD format structure files to illustrate the input described above in sections ***General rules (SSD files)*** and ***Detailed data format (SSD files)***.

(a) Clean substrate structure : Pd(100)-(1x1)

```
##
#c created 03-17-1998
"s1:Pd(100)-(1x1)"
"s2:46.12"
"s3:new in SSD3"
"s4:LEED"
"s5:J. Burchhardt, E. Lundgren, M.M. Nielsen, J.N. Andersen"
"s5:and D.L. Adams"
"s6:Surf. Rev. Lett."
"s7:3"
"s8:1339"
"s9:1996"
"s10:Pd"
"s11:fcc"
"s12:(100)"
"s13:p4m"
"s14:p4m"
"s17:(1x1)"
#ta
         1         0         0         1
#fa
"s22:320K"
"s23:multilayer relaxation: expansion of top interlayer spacing"
"s24:by 0.09\+0.03\A = 4.5\+1.5%"
"s28:prior to LEED measurements, surface was flashed to"
"s29:850K to eliminate H (which desorbs at 360K)"
"s33:elemental"
"s34:metal"
"s35:non-reconstructed"
"s38:1a.1b.1"
"t1:1"
"t2:ion bombardment followed by annealing"
"t3:sharp LEED pattern"
"t4:AES"
"t5:C <5% ML"
"t6:rear-view, video LEED"
"t7:IV spectra for 5 non-equivalent beams at normal incidence:"
"t8:E range 40-490eV"
"t9:dynamical LEED: 14 ph shs from Moruzzi et al pot;"
"t10:vibrations (layer dependent), Vo, Voi fit"
"t11:fit of top 3 interlayer spacings"
"t16:chi^2=0.035"
#tb
    2.7510     .0000     .0000    2.7510   90.0000
   1
#fb
#te
    1.9452
   5
```

```
epir      -2                  .0000A     .0000A     .0000

subr      -1                 1.3755A    1.3755A    1.9453

intf Pd    1   b 1.000   0     .0000A     .0000A     .0000     .0000

intf Pd    2   b 1.000   0    1.3755A    1.3755A    2.0400     .0000
                                                     .0300
intf Pd    3   b 1.000   0     .0000A     .0000A    3.9900     .0000
                                                     .0100
intf Pd    4   b 1.000   0    1.3755A    1.3755A    5.9200     .0000
                                                     .0200
subl Pd    5   b 1.000   0     .0000A     .0000A    7.8700     .0000

#fe
#c
"b1:bond distances and angles are derived from coordinates"
#tf
   4
    2.8188         Pd1         Pd2         Pd3   91.4318
    2.7544         Pd2         Pd3         Pd4   89.8444
    2.7402         Pd3         Pd4         Pd5   89.8444
    2.7544         Pd4         Pd5         Pd4     .0000
#ff
```

(b) Adsorbate structure with surface alloying: Al(111)-(√3x√3)R30°-Li

```
##
#c created 03-17-1998
"s1:Al(111)+(\R3x\R3)R30\0-Li"
"s2:13.3.1"
"s3:new in SSD3"
"s4:LEED"
"s5:M.M. Nielsen, S.V. Christensen and D.L. Adams"
"s6:Phys. Rev."
"s7:B54"
"s8:17902"
"s9:1996"
"s10:Al"
"s11:fcc"
"s12:(111)"
"s13:p3m1"
"s14:p31m"
"s15:Li"
"s16:1/3 Li/Al"
"s17:(\R3x\R3)R30\0"
#ta
    1.0000    1.0000   -2.0000    1.0000
#fa
"s22:100K"
"s23:adatoms in substitutional sites in top Al layer"
"s33:elemental"
"s34:metal"
"s35:reconstructed"
"s36:atomic"
"s37:substitutional"
```

```
"s38:1b.1a.3"
"t1:1"
"t2:Li depos. at 300K"
"t3:LEED: sharp spots, low background"
"t4:AES, XPS, TPD"
"t5:AES: C < 0.03ML"
"t6:video LEED"
"t7:IV spectra for 14/29 symm.-ineq. beams at \t=0/15\0;"
"t8:E range 40-400eV"
"t9:dynamical LEED (layer doubling): 14 ph shs from Moruzzi et"
"t10:al pots; rms vibs fitted for Li, Al in 1st, 2nd, bulk layers"
"t11:adsorption in fcc hollow, hcp hollow, top and substitutional"
"t12:in-top-layer sites; for substitutional site, fitting of top"
"t13:4 interlayer spacings, and lateral position of 2nd Al layer"
"t16:chi^2=0.033"
#tb
    2.8525     .0000    1.4262    2.4703   60.0005
   1   1
#fb
"2d8:s1"
#tc
    4.2787    2.4703   -4.2788    2.4703  120.0008
#fc
"2d14:(\R3x\R3)R30\0"
#td
    1.0000    1.0000   -2.0000    1.0000
#fc
"3d1:Li1: adatom in substitutional site;"
"3d2:Al2-3: remaining Al atoms of top Al layer"
#te
    2.3291
   7
epir      -2                   .0000A     .0000A     .0000

subr      -1                   .0000A    1.6470A    2.3291

ovrl Li    1  s1  .333   0     .0000f     .0000f     .0000     .0000

intf Al    2  s1  .333   1     .6667f     .3333f     .4100     .0000
                                                    .1000
intf Al    3  s1  .333   2    -.3333f     .3333f     .0000     .0000

intf Al    4   b 1.000   3     .6667f    -.3333f    2.2900     .0000
                             .0100f     .0100f     .0200
intf Al    5   b 1.000   4     .6667f    -.3333f    2.3100     .0000
                                                    .0200
intf Al    6   b 1.000   5    -.3333f    -.3333f    2.3300     .0000
                                                    .0200
subl Al    7   b 1.000   6    -.3333f    -.3333f    2.3291     .0000

#fe
#c
"b1:bond distances and angles are derived from coordinates"
#tf
   4
    2.8819         Li1         Al2         Al3   60.3315
    3.1627         Li1         Al4         Al5  122.9632
```

```
    2.8522         Al2         Al3         Al4   59.6232
    2.8204         Al2         Al4         Al5  119.4492
#ff
```

(c) Structure of epitaxial thin film on metal substrate: Pd(100)+(1x1)-multilayer-bct-Co(100)-(1x1)

```
##
#c created 03-17-1998
"s1:Pd(100)+(1x1)-multilayer-bct-Co(100)-(1x1)"
"s2:46.27.1"
"s3:new in SSD3"
"s4:XPD"
"s5:H. Giordano, A. Atrei, M. Torrini, U. Bardi, M. Gleeson and"
"s5:C.J. Barnes"
"s6:Phys. Rev."
"s7:B54"
"s8:11762"
"s9:1996"
"s10:Pd"
"s11:fcc"
"s12:100"
"s13:p4m"
"s14:p4m"
"s15:Co"
"s16:2-35 ML"
"s17:(1x1)"
#ta
         1         0         0         1
#fa
"s22:300K"
"s23:metastable pseudomorphic Co film distorted from fcc to bct"
"s24:by a large expansion of the in-plane lattice parameter and a"
"s25:10% contraction of the interlayer spacing;"
"s26:this structure persists to thicknesses of the film larger"
"s27:than 30 layer equivalents; 3ML case is tabulated here"
"s33:elemental"
"s34:metal"
"s35:non-reconstructed"
"s36:atomic"
"s37:pseudomorphic"
"s38:1e.1b.1"
"t1:1"
"t2:cycles of Ar+ sputtering and annealing"
"t3:LEED: sharp spots"
"t4:XPS"
"t5:Carbon <0.1 ML"
"t6:XPS Co 2p intensity vs. emission angles"
"t7:polar XPD curves for Co 2p3/2 peak measured at 2"
"t8:non-equivalent azimuths for various Co coverages"
"t9:Single Scattering Cluster"
"t10:Spherical Wave (SSC-SW) theory"
"t11:fcc structure of the Co film with distortions of the"
"t12:in-plane parameter (2.55-2.95 \A) and of the interlayer"
"t13:distance (1.4-1.8 \A); calculations were performed for"
"t14:3 ML on Pd(100) and infinitely thick Co films"
"t16:visually good"
```

```
#tb
    2.7500     .0000     .0000    2.7500   90.0000
   1   1
#fb
"2d8:s1"
#tc
    2.7500     .0000     .0000    2.7500   90.0000
#fc
#td
         1         0         0         1
#fc
"3d1:Co1-3: bct pseudomorphic film"
#te
    1.9440
   4
epir      -2                   .0000f     .0000f     .0000

subr      -1                  1.3750f    1.3750f    1.9440

ovrl Co    1  s1 1.000   0     .0000f     .0000f     .0000     .0000
                               .0000f     .0000f     .0500
ovrl Co    2  s1 1.000   0     .5000f     .5000f    1.5500     .0000
                               .0000f     .0000f     .0500
ovrl Co    3  s1 1.000   0     .0000f     .0000f    3.1000     .0000
                               .0000f     .0000f     .0500
subl Pd    4   b 1.000   0     .5000f     .5000f    5.0440     .0000
                               .0000f     .0000f     .0000
#fe
#c
"b1:bond distances and angles are derived from coordinates"
#tf
   2
    2.4867         Co1         Co2         Co1     .0000
    2.7496         Pd4         Co3         Pd4     .0000
#ff
```

Technique abbreviations

AED	Auger Electron Diffraction
AFM	Atomic Force Microscopy
ALISS	Alkali Ion Scattering Spectroscopy
ALICISS	Alkali ICISS
ARAES	Angular Resolved Auger Electron Spectroscopy
ARPES	Angular Resolved Photoelectron Spectroscopy
ARUPS	Angular Resolved Ultraviolet Photoelectron Spectroscopy
ARXPS	Angular Resolved X-ray Photoelectron Spectroscopy
ARXPD	Angular Resolved X-ray Photoelectron Diffraction
ARPEFS	Angular Resolved Photoelectron Fine Structure
At. diffr.	Atom Diffraction
ATLEED	Automated Tensor LEED
At. scatt.	Atom Scattering
BSN	Beam-Set Neglect
CAICISS	Coaxial Impact-Collision Ion Scattering Spectroscopy
CMA	Cylindrical Mirror Analyzer
CMTA	Constant-Momentum Transfer Averaging
CSM	Combined Space Method
CWMS	Curved-Wave Multiple Scattering
DLEED	Diffuse LEED
EAPFS	Electron Appearance Potential Fine Structure
EELFS	Electron Energy Loss Fine Structure
EELS	Electron Energy Loss Spectroscopy
EH	Electron Holography
EM	Electron Microscopy
ESDIAD	Electron Stimulated Desorption Ion Angular Distribution
EXAFS	Extended X-ray Absorption Fine Structure
EXELFS	Extended Electron Energy Loss Fine Structure
EXFAS	Extended Fine Auger Structure
FIM	Field Ion Microscopy
Fluorescence XRD	Fluorescence X-ray Diffraction
FYNES	Fluorescence-Yield Near-Edge Structure
GIXD	Grazing-Incidence X-ray Diffraction
GIXS	Grazing-Incidence X-ray Scattering
He diffr.	Helium Diffraction
HEIS	High-Energy Ion Spectroscopy
HREELS	High-Resolution Electron Energy Loss Spectroscopy
ICISS	Impact Collision Ion Scattering Spectroscopy
INS	Ion Neutralization Spectroscopy
Ion scatt.	Ion Scattering
IRS, IRAS	Infrared (Reflection-Absorption) Spectroscopy
ISS	Ion Scattering Spectroscopy

KLEED	Kinematic Low-Energy Electron Diffraction
KSLA	Kinematic Sublayer Addition
LEIS	Low-Energy Ion Spectroscopy
LEED	Low-Energy Electron Diffraction
LEPD	Low-Energy Positron Diffraction
MEED	Medium-Energy Electron Diffraction
MEIS	Medium-Energy Ion Spectroscopy
MEIS-SB	MEIS with Shadowing and Blocking
Neutr. diffr.	Neutron Diffraction
NEXAFS	Near-Edge X-ray Absorption Fine Structure
NMR	Nuclear Magnetic Resonance
NPD	Normal Photoelectron Diffraction
OPD	Off-normal Photoelectron Diffraction
PED	Photoelectron Diffraction
PES	Photoelectron Spectroscopy
PEXAFS	Photoemission Extended X-ray Absorption Fine Structure
PLEED	(Spin-) Polarized LEED
QDLEED	Quasi-Dynamic Low-Energy Electron Diffraction
QKLEED	Quasikinematical Low-Energy Electron Diffraction
RAIRS	Reflection-Absorption Infrared Spectroscopy
RBS	Rutherford Backscattering
RFS	Renormalized Forward Scattering
RHEED	Reflection High-Energy Electron Diffraction
RSP	Reverse Scattering Perturbation
SEELFS	Surface Electron Energy Loss Fine Structure
SEM	Scanning Electron Microscopy
SEXAFS	Surface Extended X-ray Absorption Fine Structure
SIMS	Secondary Ion Mass Spectroscopy
SPLEED	Spin-Polarized LEED
SSRL	Stanford Synchrotron Radiation Laboratory
STM	Scanning Tunneling Microscopy
TDS	Thermal Desorption Spectroscopy
TEAS	Thermal Energy Atomic Scattering
TED	Transmission Electron Diffraction
TEM	Transmission Electron Microscopy
TLEED	Tensor LEED
TOF-SARS	Time-of-Flight Scattering and Recoiling Spectroscopy
TPD	Temperature Programmed Desorption
Transm. Channeling	Transmission Channeling
UPS	Ultraviolet Photoelectron Spectroscopy
WF(C)	Work Function (Change)
XAFS	X-ray Absorption Fine Structure
XANES	X-ray Absorption Near-Edge Structure

XAS	X-ray Absorption Spectroscopy
XPD	X-ray Photoelectron Diffraction
XPS	X-ray Photoelectron Spectroscopy
XRD	X-ray Diffraction
XSW	X-ray Standing Wave

Journal abbreviations

Acta Crys.	Acta Crystallographica
Appl. Phys.	Applied Physics
Appl. Surf. Sci.	Applications of Surface Science
Can. J. Chem.	Canadian Journal of Chemistry
Can. J. Phys.	Canadian Journal of Physics
Chem. Phys.	Chemical Physics
Chem. Phys. Lett.	Chemical Physics Letters
Europhys. Lett.	Europhysics Letters
J. Am.Chem. Soc.	Journal of the American Chemical Society
Jap. J. Appl. Phys.	Japanese Journal of Applied Physics
J. Chem. Phys.	Journal of Chemical Physics
J. Phys.	Journal of Physics (London)
J. Phys. Chem.	Journal of Physical Chemistry
J. Phys. CM	Journal of Physics (London) - Condensed Matter
J. Vac. Sci. Technol.	Journal of Vacuum Science and Technology
Langmuir	(not abbreviated)
Phys. Lett.	Physics Letters
Phys. Stat. Sol.	Physica Status Solidi
Phys. Rev.	Physical Review
Phys. Rev. Lett.	Physical Review Letters
S. Afr. J. Phys.	South African Journal of Physics
Solid State Commun.	Solid State Communications
Springer Series in Surface Sciences	(not abbreviated)
Surf. Rev. Lett.	Surface Review and Letters
Surf. Sci.	Surface Science
Vacuum	(not abbreviated)
Zeitschrift f. Kristallographie	(not abbreviated)
Z. Phys.	Zeitschrift für Physik
Z. Naturf.	Zeitschrift für Naturforschung

Table of 2D Space Groups

The following table gives all **17** 2-dimensional **space groups** together with their nomenclature in SSDIN. The numbering scheme is identical to that used in the International Tables for X-ray Crystallography (Ref. 5 of the ***Bibliography***). The space group type is listed in both full and short notation.

Number	type	class	SSDIN name
1	p1	oblique	‘‘[1] Oblique p1’‘
2	p211 (p2)	‘‘	‘‘[2] Oblique p2’‘
3	p1m1 (pm)	primitive rectangular	‘‘[3] Primtv. Rect. pm’‘
4	p1g1 (pg)	‘‘	‘‘[4] Primtv. Rect. pg’‘
5	c1m1 (cm)	centered rectangular	‘‘[5] Centrd. Rect. cm’‘
6	p2mm (pmm)	primitive rectangular	‘‘[6] Primtv. Rect. p2mm (pmm)’‘
7	p2mg (pmg)	‘‘	‘‘[7] Primtv. Rect. p2mg (pmg)’‘
8	p2gg (pgg)	‘‘	‘‘[8] Primtv. Rect. p2gg (pgg)’‘
9	c2mm (cmm)	centered rectangular	‘‘[9] Centrd. Rect. c2mm (cmm)’‘
10	p4	square	‘‘[10] Square p4’‘
11	p4mm (p4m)	‘‘	‘‘[11] Square p4mm (p4m)’‘
12	p4gm (p4g)	‘‘	‘‘[12] Square p4gm (p4g)’‘
13	p3	hexagonal	‘‘[13] Hexagonal p3’‘
14	p3m1	‘‘	‘‘[14] Hexagonal p3m1’‘
15	p31m	‘‘	‘‘[15] Hexagonal p31m’‘
16	p6	‘‘	‘‘[16] Hexagonal p6’‘
17	p6mm (p6m)	‘‘	‘‘[17] Hexagonal p6mm (p6m)’‘
(3')*	pm'	primitive rectangular	‘‘[3'] Rot. Prim. Rect. pm’‘
(4')*	pg'	‘‘	‘‘[4'] Rot. Prim. Rect. pg’‘
(5')*	cm'	centered rectangular	‘‘[5'] Rot. Cent. Rect. cm’‘
(6')*	p2mg' (pmg')	primitive rectangular	‘‘[7'] Rot. Prim.Rect. p2mg (pmg)’‘

* For some superlattices, space groups [3], [4], [5], [7] of the superlattice can appear with two inequivalent orientations of their mirror and glide planes. Examples are p(2x1) or c(4x2) on p6mm. In these cases, LEEDpat includes the rotated groups as [3'], [4'], [5'], [7']. These rotated groups can also be used to rotate the orientation of mirror and glide planes in other situations, where they are equivalent under rotation, e.g. for p(2x1) on p4mm.

The following list shows all symmetry elements present in each space group.

Space group	symmetry elements
[0] none	for disordered, non-periodic surface structures
[1] p1	oblique cell, no point symmetry
[2] p2	oblique cell, 2-fold rotation axis
[3] pm	primitive rectangular cell, 1 mirror plane
[4] pg	primitive rectangular cell, 1 glide plane
[5] cm	centered rectangular cell, 1 mirror plane, 1 parallel glide plane
[6] pmm	primitive rectangular cell, 2 orthogonal mirror planes, 2-fold rotation axis

[7] pmg	primitive rectangular cell, 1 mirror plane, 1 orthogonal glide plane, 2-fold rotation axis
[8] pgg	primitive rectangular cell, 2 orthogonal glide planes, 2-fold rotation axis
[9] cmm	centered rectangular cell, 2 orthogonal mirror planes, 2 orthogonal glide planes, 2-fold rotation axis
[10] p4	primitive square, 4-fold rotation axis, 2-fold rotation axis
[11] p4m	primitive square, 2 orthogonal mirror planes, 2 orthogonal glide planes (diagonally), 4-fold rotation axis, 2-fold rotation axis
[12] p4g	primitive square, 2 orthogonal mirror planes, 2 orthogonal mirror planes (diagonally), 4-fold rotation axis, 2 orthogonal glide planes, 2-fold rotation axis
[13] p3	primitive hexagonal, 3-fold rotation axis
[14] p3m1	primitive hexagonal, 3 mirror planes (orthogonal to sides), 3 glide planes (orthogonal to sides), 3-fold rotation axis
[15] p31m	primitive hexagonal, 3 mirror planes (parallel to sides), 3 glide planes (parallel to sides), 3-fold rotation axis
[16] p6	primitive hexagonal, 6-fold rotation axis, 2-fold rotation axis
[17] p6m	primitive hexagonal, 6 mirror planes, 6 glide planes, 6-fold rotation axis, 2-fold rotation axis

---

Note on p3m1 vs. p31m: these differ in the orientation of the mirror (and glide) planes, which are rotated by 30 degrees in going from p3m1 to p31m, or vice versa; p3m1 applies to clean non-reconstructed fcc(111), bcc(111), hcp(0001) and similar surfaces; p31m applies to such substrates with simple adsorbates in 3-fold symmetrical adsorption sites for supercells like $(\sqrt{3}x\sqrt{3})R30°$; each case should be checked individually.

Bulk / interlayer spacing

The ‘‘Bulk substrate interlayer spacing’‘ is used as a reference spacing in setting up the final SSD database entries: it is meant to express the interlayer spacings **relative** to the bulk value in the substrate (i.e. expressed in %, such that 100% implies a spacing equal to that in the substrate bulk). This is particularly useful to exhibit deviations from the bulk interlayer spacing near the surface. You only input the ‘‘Bulk substrate interlayer spacing‘‘ and SSDIN does the rest automatically.

Typically, this ‘‘Bulk substrate interlayer spacing‘‘ is the bulk layer-to-layer repeat distance in the case of simple substrates. It is often equal to the z-component of the ‘‘Substrate bulk 3D repeat vector’‘, but there are a number of exceptions. Examples:

- for **fcc(100)** one would choose a/2 (if a is the bulk cube edge)
- for **hcp(0001)** one would choose c/2 (if c is the hcp lattice constant perpendicular to the basal plane, such that c is twice the interlayer spacing in that direction, while in this hcp case ‘‘Substrate bulk 3D repeat vector‘‘ would have c as z-component)
- for Si(111) one could choose the bilayer-to-bilayer repeat spacing, rather than the smaller interlayer spacings that exist between adjacent monolayers: both choices are valid

Region

A surface or interface is divided into up to 4 ‘‘regions’‘, namely ‘‘substrate’‘, ‘‘interface’‘, ‘‘overlayer’‘, and ‘‘epilayer’‘, abbreviated as ‘‘subl‘‘, ‘‘intf‘‘, ‘‘ovrl‘‘, and ‘‘epil‘‘, resp. Each atom belongs to a specific region. The regions are defined as follows:

subl: substrate. The atoms labeled ‘‘subl‘‘ repeat indefinitely into the substrate according to the ‘‘Substrate bulk 3D repeat vector‘‘ (see ***Definition of 3D repeat vectors***). For a substrate bulk with one atom per primitive 3D unit cell, only one layer labeled ‘‘subl‘‘ is needed, e.g., for fcc and bcc. For a substrate bulk with N atoms per 3D primitive unit cell, N layers labeled ‘‘subl‘‘ are needed: e.g., N=2 for hcp, diamond, zincblende and wurtzite, and N=4 for graphite. The atoms labeled ‘‘subl‘‘ are assumed to form a group of layers that will be repeated together to form the semi-infinite substrate. The relative coordinates specified for these atoms must therefore be substrate-bulk-like, i.e. no relaxations may be present that would be repeated into the bulk.

intf: interface. This typically represents surface-relaxed substrate atoms at the interface between bulk and vacuum. Atoms of this type can also form underlayers (in the case of compound formation), or be relaxed atoms at a substrate-epilayer interface.

ovrl: overlayer. Such atoms are typically foreign adatoms or admolecules. (The distinction between interface and overlayer atoms may not always be clear-cut, leaving a choice in labeling.) They may also be relaxed epilayer atoms at an interface.

epil: epilayer. The atoms labeled ‘‘**epil**‘‘ repeat indefinitely into the epilayer, according to the ‘‘Epilayer bulk 3D repeat vector‘‘(see ***Definition of 3D repeat vectors***). Their meaning is directly analogous to that of ‘‘subl‘‘ layers, but for a semi-infinite epilayer extending away from the substrate-epilayer interface. When two or more atoms are labeled ‘‘epil‘‘, they are assumed to form a group of layers that will be repeated together into the epilayer. The relative coordinates specified for these atoms are thus epilayer-bulk-like.

Definition of 3D repeat vectors

SSD represents the **bulk** of the substrate as a **semi-infinite repeating 3D lattice**. It is defined by a so-called **‘‘substrate bulk 3D repeat vector’‘**, which, when applied to a set of one or more bulk-like layers, generates the substrate to infinite depth. (These bulk-like layers will be later defined by the region type ‘‘subl’‘.)

When describing an **interface** between a substrate and an epilayer (a relatively rare occurrence so far in SSD), that **epilayer** is treated in much the same way: as a **semi-infinite bulk** described by a so-called **‘‘epilayer bulk 3D repeat vector’‘** and one or more bulk-like layers of the epitaxial material (later labeled by the ‘‘region’‘ type ‘‘epil’‘). This vector should be left blank if the structure does not contain an epilayer.

Note: substrate and epilayer bulk 3D **repeat vectors** point in the direction **toward their bulk volume**, i.e. the **z** component of the **substrate** repeat vector must be **positive**, that of the **epilayer** repeat vector must be **negative**.

Site occupancy

‘‘Site occupancy’‘ gives, for ordered and incommensurate layers, the coverage of a layer with respect to the substrate (1x1) cell. Thus, a (2x1) layer typically has a site occupancy of 0.5, while (2x2) gives 0.25. For a displacive reconstruction (which breaks the periodicity of a layer into a larger unit cell by displacements such as out-of-plane bucklings), this occupancy will be <1, e.g., 0.5 for each of the two atoms defining a c(2x2) buckled layer. (**Note** that the two atoms in this example must be tabulated separately).

For non-reconstructive disordered layers (type ndk), the ‘‘Site occupancy’‘also gives the coverage of a layer with respect to the substrate (1x1) cell. Thus, if you specify a cell ‘‘nd1’‘ that is simply a (1x1) cell, then atoms will randomly occupy the same site within each (1x1) cell on the surface, with a probability given by the site occupancy. This is the most common situation.

One complication that can occur with disordered layers defined on a (1x1) lattice is an overlap between large neighboring adsorbates: e.g. a C6H6 molecule can cover several (1x1) cells. To avoid this overlap, the adsorbates may be forced apart by defining an artificial superlattice on which these large adsorbates are located, with random probability.

Another case is a disordered layer residing at sites on a superlattice (such as on a reconstructed substrate): these atoms must also be located on such a superlattice, with random probability.

In all these cases, the ‘‘Site occupancy’‘ still is the coverage relative to a (1x1) cell.

For the lattice types rdk (reconstructive lattice-gas disorder) and mk (randomly mixed layer), the ‘‘Site occupancy’‘ is the experimentally determined or estimated coverage or fraction, rather than the value appropriate for the artificial periodic structure representing it in SSD. For instance, if a disordered overlayer of 0.2 coverage is modeled as a (2x2) overlayer of type rdk because it induces substrate relaxations, the site occupancy is given as 0.2 and not 0.25.

Bibliography and downloads

[1] P. R. Watson, M. A. Van Hove and K. Hermann, *NIST Surface Structure Database Ver. 5.0*, NIST Standard Reference Data Program, Gaithersburg, MD, USA (2004).

[2] J. B. Pendry, *Low-Energy Electron Diffraction*, Academic Press, London, 1974.

[3] M. A. Van Hove and S. Y. Tong, *Surface Crystallography by LEED*, Springer Verlag, Heidelberg, 1979.

[4] M. A. Van Hove, W. H. Weinberg, and C.-M- Chan, *Low-Energy Electron Diffraction, Experiment, Theory and Surface Structure Determination*, Springer Series in Surface Science, Vol. 6, G. Ertl and R. Gomer (Eds.), Springer Verlag, Heidelberg, 1986 (out of print).

[5] International Tables for X-ray Crystallography, Vol. I Symmetry Groups, eds. N.F.M. Henry and K. Lonsdale, Kynoch Press (Birmingham, England), 1965, pp. 6, 45-47, 57-72.

[6] E. A. Wood, J. Appl. Phys. 35, 1306 (1964).

[7] Useful web sites and downloads

SSD, Surface Structure Database V. 5 (WIN95/98/NT/2k/XP/Vista/7) :
http://www.nist.gov/srd/nist42.htm (database, V. 5)
http://www.fhi-berlin.mpg.de/KHsoftware/ssdin5/index.html (structure input, visualizer, V. 5)
SURFACE EXPLORER, surface visualization (web application) :
http://surfexp.fhi-berlin.mpg.de
LEEDpat, LEED symmetry pattern simulator (WIN95/98/NT/2k/XP) :
http:// www.fhi-berlin.mpg.de/KHsoftware/LEEDpat/index.html
BALSAC, surface visualization, design, and analysis (DOS, WIN95/98/NT/2k/XP, Unix) :
http://www.fhi-berlin.mpg.de/KHsoftware/Balsac/balpam.html (pamphlet)
http://www.fhi-berlin.mpg.de/KHsoftware/Balsac/Balsac3.pdf (manual)
http://www.fhi-berlin.mpg.de/KHsoftware/Balsac/pictures.html (picture gallery)
SARCH/LATUSE/PLOT3D, surface visualization, and analysis (DOS, outdated) :
http://www.fhi-berlin.mpg.de/KHsoftware/SLP/index.html

About SSDIN, SSD

The **Surface Structure Database INput Preparation (SSDIN), Version 5,** software was developed by Klaus Hermann (Fritz-Haber-Institut Berlin, Germany) in collaboration with Phillip R. Watson (Oregon State University, Corvallis, USA) and Michel A. Van Hove (formerly Lawrence Berkeley National Laboratory, Berkeley, USA; now Dept. of Physics and Materials Science, City University of Hong Kong (SAR)), and the National Institute of Standards and Technology (NIST, Gaithersburg, MD, USA).

SSDIN forms a supplement of the **Surface Structure Database (SSD)**, Version 5 and higher, NIST Database No. 42. Version 4.0 of SSD was published in electronic form in 2001 and distributed by NIST (see http://www.nist.gov/srd/nist42.htm for further information). It includes surface structures published until January 2000, totalling about 1300 structure determinations. The SSDIN software is meant to assist researchers in preparing their structure information for submission to the authors of SSD.

The **SSD format**, also called **ASD** (ASCII Structure Data) format, has been developed for archiving detailed surface structure data for inclusion in the NIST Surface Structure Database (SSD) by Michel A. Van Hove.

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