Critical Compilation of Surface Structures Determined by Ion Scattering Methods

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Critical Compilation of Surface Structures Determined by Ion Scattering Methods

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This review critically compiles all surface structures derived by ion scattering techniques reported in the refereed literature prior to January 1988. They are compared with the more extensive low-energy electron diffraction database reported previously [J. Phys. Chem. Ref. Data 16, 953 (1957)]. These investigations cover all types of surfaces including clean and adsorbate-covered metal, semiconductor, and other nonmetallic substrates. The important experimental and theoretical aspects of such investigations have been extracted into easily understood tabular form supplemented by many figures and ancillary tables and complete references. It is hoped that this compilation will provide a valuable resource both for the surface science specialist and for those nonspecialists in other areas who need surface crystallographic data.

Key words: critically reviewed data; ion scattering; channelling; blocking; surface crystallography; surface structure.

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1. Introduction

1.1. Background

urfaces play an increasingly important role in technol-1 the construction of microelectronics circuits, the acf catalysts, and in the areas of metallurgy, tribology, prrosion. Many of the most dramatic advances in these have resulted from the application of the methods of e science.

'he geometrical arrangement of atoms in a surface or ed layer is perhaps the single most basic item of infor-1 that we need in order to understand the behavior of rfaces of materials. From the surface crystallography, t all other understanding flows. Thus, a knowledge of e structure is a prerequisite for studies of electronic ties. Without surface crystallographic information,

attempts to define adsorption and reactions on surfaces are critically hindered.

A number of techniques that are sensitive to the atomic geometry of surfaces have been developed, using electron, 103 photon, and ion probes. The most widely-used of these has been low-energy electron diffraction (LEED), which was the subject of a previous critical compilation.¹ Of the other methods, ion scattering studies have provided the most in-104 formation on surface crystallography.

Unlike the LEED literature, which contains several lists of derived structures, there have been few attempts to compile an overview of the results from ion scattering, critical or otherwise. However, several interesting reviews exist. The most comprehensive is that of van der Veen² which pro-108 vides a good review of the principles of high- and mediumenergy scattering, and discussion of applications to surfaces and interfaces up to 1984. The present compilation provides a greater depth of detail of a wider range of investigations, including low-energy studies, and brings the listing up to date. In particular we provide a survey of surface structural results that has been critically examined as to the accuracy 100 and internal consistency of the quoted results. The present compilation summarizes in detail the ion-scattering surface crystallography literature in a condensed, but easily accessible, database. In addition, the results are discussed and compared with existing LEED structures. It is hoped that this 102 survey will be a valuable resource not only for specialists in surface science, but also for workers in other disciplines that need surface structural data to understand and extend their work, but lack the time or resources to evaluate the complex and interrelating factors that contribute to the derivation of a structure quoted in the literature.

1.2. Organization and Scope

The body of the review is organized as follows. First we very briefly review the basic aspects of ion scattering experiments to orient those readers not familiar with this topic. More complete accounts can be found in the reviews referred to therein. Next we examine in some detail the various components that go into a surface structural determination by these methods and attempt to establish criteria that would give us a reasonable degree of confidence in the derived result.

The compilation of surface structures is presented in the form of a large table (Table 2), showing the most important experimental and theoretical parameter values and a brief description of the results of the study. Further discussion of some of the reported structures follows in Sec. 5, and is divided into three sections covering: (1) Clean surfaces of metals and alloys, (2) adsorbate-covered metal surfaces, and (3) nonmetallic surfaces, clean and adsorbate covered. Each discussion section contains a number of accompanying notes, figures, and ancillary tables. These serve to amplify and clarify the brief descriptions given in the main table. Where possible we compare the ion scattering results with well-established LEED structures. However, in the interests of brevity, we do not fully discuss the LEED data, only the best-accepted results. Readers who require more information on LEED surface crystallographic structures are urged to refer to the previous compilation,¹ and references therein.

The temporal scope of this review covers surface structures determined by ion scattering methods reported in the refereed literature since the inception of modern investigations, roughly 1975, until January 1988.

The scope has also been deliberately limited in other ways. The first is that in order to ensure the reliability of the compilation, only papers appearing in normal peer-reviewed journals were considered; articles published in unrefereed conference proceedings or society bulletins are not included. Secondly, the review is restricted as much as is feasible to "true surface structures"-that is, to studies that result in the finding of the atomic coordinates of atoms in the first few atomic layers of a solid. This approach provides a natural continuity with the previous compilation. Hence, investigations dealing with the structure of buried interfaces, or defects in thin films, are excluded. As these problems are becoming increasingly common goals in ion scattering, particularly for channelling experiments, this exclusion may lead some readers to the mistaken impression that the review is missing recent references. Thirdly, where the same group of investigators has reported several times on the same structural problem (perhaps in increasing levels of detail), the results have been consolidated into one table entry. However, in such cases all the references are supplied.

2. Surface Structural Techniques

2.1. Introduction

There are many techniques available that are sensitive to one or another structural aspect of a surface. For the purposes of this review we shall not use the term "structure" to mean a completely determined geometry, in the sense that an x-ray crystallographer might understand the term. Surface crystallography has not advanced to that highly automated level of development. Rather we interpret "structure" in the broadest sense to mean a report of a surface geometry that may be fragmentary and incomplete, but still advances our understanding of the system.

The previous compilation¹ was concerned with the large database of LEED structures. Other surface structural techniques have been applied to a smaller range of materials. Of these, the ion-scattering spectroscopies, in their low-, medium-, and high-energy versions, have supplied the major fraction of the reported structures.

2.2. Ion Scattering Methods

Surface structure determinations using ion scattering have tended to become grouped into three types, depending upon the energy regime of the probe ion—low, medium, or high. The distinction between medium- and high-energy scattering, is in many ways an artificial one, based more upon different experimental requirements than substantial differences in the physics of the interactions.

Low-energy ion scattering (LEIS) experiments generally use ion energies of up to a few keV, and can be distinguished from the medium-energy counterpart (MEIS), in which energies are measured in 10's or 100's of keV. The distinction between medium- and high-energy scattering (HEIS) is less firm on energetic grounds. High-energy experiments usually employ MeV beams, but may drop substantially below this, while some MEIS experiments may use energies as high as 300 keV. However, the spirit of the experiments, and the apparatus used, is usually rather different for the two regimes. For the purposes of this review, we shall make the following arbitrary energetic dividing lines between the three scattering methods: (1) Low energy (LEIS): <10 keV; (2) Medium energy (MEIS): 10 keV-250 keV; (3) High energy (HEIS): >250 keV.

The physics of the interactions of ions with surfaces is simpler, at least in the energy ranges for HEIS and MEIS, than that for low-energy electrons. Furthermore, the ion scattering techniques directly determine atomic positions in real, rather than reciprocal, space. The interpretation of HEIS and MEIS spectra are more straightforward than the corresponding LEED data. As a result useful information, such as adsorbate locations, can frequently be found almost by inspection. For the most accurate HEIS and MEIS crystallographic work, significant calculations are needed, which can rival those necessary in LEED.

In the following sections we will very briefly review the essentials of ion scattering experiments in each regime.

2.2.a. High-Energy Ion Scattering (HEIS)

High-energy ion scattering is a surface-sensitive variant of the frequently used technique, Rutherford backscattering spectrometry (RBS). When the first attempts to apply RBS to surface structure determinations were performed about 15 years ago, the method already had a long history as a thinfilm analytical tool.³ A number of excellent reviews of HEIS exist,^{2,4-9} although most concentrate on experimental methods and theory, rather than a comprehensive list of results.

In a typical HEIS experiment a collimated MeV beam of ions, often He or H, is incident on a planar sample and a solid-state nuclear particle detector measures the scattered particles. If the ion beam is carefully aligned along a major symmetry direction of the crystal, most of it is then channeled in this direction by the atom strings of the solid; the ions cannot approach close enough to undergo large-angle Rutherford scattering. As a result the signal from the bulk of the solid is dramatically reduced. The surface atoms are always accessible to the ion beam, and so the surface peak (SP) becomes clearly separated in the energy spectrum.

When ions scatter from the surface layer of the solid they project a "shadow-cone" within which scattering from atoms in deeper layers is suppressed. In an ideal lattice, the size of the SP is related to the relative sizes of the two-dimensional thermal vibration amplitude, and the radius of the shadow cone. One of the great strengths of HEIS is that the response of the SP to different surface structures can be predicted in a simple geometrical manner.

Obtaining detailed crystallography involves calculating the SP expected for a particular postulated surface structure. The nuclear backscattering probability is determined by a Monte Carlo approach⁹⁻¹² in which a large number of trajectories of ions in the crystal are followed. The interaction potential is frequently of the screened Coulomb type due to oliere.¹³ The other main input to the calculations are the brational amplitudes of the surface and near-surface oms, which are not known *a priori*. Recent work has exored the effect of correlated atomic motions on the SP.¹⁴ ne lack of information on vibrational properties of surface oms may ultimately limit the accuracy of structural deterination by ion scattering methods.

The form in which data is collected and analyzed is ually of two main types: (1) The SP intensity is measured a certain channeling direction, and at a number of ion lergies, and the resulting experimental SP/energy curve ted to calculations. (2) A "rocking-curve" consisting of e SP intensity as a function of small changes of angle about e channelling direction is compared with theory.

The extraction of the SP intensity is sensitive to the ethod of background subtraction.¹¹

The angular and/or energy data is then compared with lculations for various assumed geometries in a trial-andror process, monitored often by a reliability (R-) factor. In intrast to LEED, and most other techniques, ion scattering oss sections can be measured and calculated in absolute, ther than relative, units. Hence, there is less need in ion attering for the complex R-factors that have been necesry in LEED to account for the arbitrariness of the ordiite. Typically, simple, statistically justifiable, R-factors ive been used for HEIS (Table 1); they are all based on ot-mean-square differences between experimental and eoretical quantities. The factors differ in the use of experiental weighting factors (RWIS¹⁸ and RIS¹⁷), and normalition (RSQ)¹⁶ as shown below:

$$RSQ = \frac{1}{N} \left[\sum_{i=1}^{N} \left[Y_{th} - Y_{ex} \right]^{2} \right]^{1/2}$$
$$RIS = \frac{100}{N} \left[\sum_{i=1}^{N} \left(\frac{\left[Y_{th} - Y_{ex} \right]}{Y_{ex}} \right)^{2} \right]^{1/2}$$
$$RWIS = 100 \frac{1}{N} \left[\sum_{i=1}^{N} \left(\frac{\left[Y_{th} - wY_{ex} \right]}{wY_{ex}} \right)^{2} \right]^{1/2}$$

Here Y_{th} and Y_{ex} are the calculated and experimental SP elds, N the number of data points, and w a weighting factor use to 1 that takes account of experimental errors.

2.2.b. Medium-Energy Ion Scattering (MEIS)

Ion scattering in the medium energy range has been extensively developed and reviewed by Dutch workers.^{2,19-21} It shares a similar conceptual base, and employs many of the same theoretical approaches as HEIS.

The critical component that most clearly differentiates most MEIS and HEIS studies is the use of "blocking" of the exiting backscattered particle in addition to channeling of the incoming ion. If a backscattering atom is located below the surface, then the outgoing scattered ion may be blocked along its exit track by another atom, resulting in a decrease in the SP in that direction.

If the sample and detector are accurately set up in "double alignment", that is, with the ion beam incident along a channeling direction, and the detector on a blocking direction, then changes in interlayer spacings can be measured from the tilt angle of the surface blocking cone with respect to the bulk axis.

The usual method of data presentation in MEIS is the surface blocking pattern. Here the intensity of the SP, for a given channeling direction, is measured about one or more blocking directions. The position and shape of the blocking minima can then be compared with calculations for assumed surface structures.²²⁻²⁴

The use of R-factors in MEIS studies has increased lately. There appears to be trend to use factors that are more securely based in statistical theory; two popular R-factors $are^{24.25}$:

$$R1v = \frac{1}{vs} \sum_{i=1}^{N} |wY_{ex} - Y_{th}|$$
$$R2v = \frac{1}{vs^{2}} \sum_{i=1}^{N} [wY_{ex} - Y_{th}]^{2}$$

where, s is the standard deviation in data values $Y(ex)_i$, N is the number of data points, v is the number of degrees of freedom = (N - the number of parameters to fit), and w is a weighting factor

2.2.c. Low-Energy Ion Scattering (LEIS)

The low-energy ions employed in LEIS interact so strongly with solid materials that scattering is almost com-

| R-factor | Application | Form ^a | Ref. |
|----------|-------------|-------------------|------|
| RSQ | HEIS | R.M.S. Th-Exp | 16 |
| RIS | HEIS, MEIS | Normalized RSQ | 17 |
| RWIS | HEIS | Weighted RIS | 18 |
| R1v | MEIS | Mean Th-Exp | 25 |
| R2v | MEIS | Similar to RWIS | 31 |
| | | | |

Table 1. Reliability (R-) factors used for ion scattering crystallography.

^a for more detail see text

pletely confined to the topmost surface layer. As a result, ion scattering spectroscopy (ISS) has found considerable use as a surface analytical tool.²⁶ As a surface structural probe, LEIS shares many of the same phenomena as MEIS or HEIS, in particular the use of blocking. But LEIS is also distinctly separated from HEIS and MEIS experiments in that quantitative analysis is much less straightforward due to a poorer understanding of the interaction potential, and a lack of knowledge of the probability of neutralization of the scattered ion. A number of reviews of various aspects of LEIS are in the literature.²⁷⁻³⁰

In LEIS, the kinematic relations for the energy of the scattered projectile remain unchanged from higher energies, at least under the assumption of two-particle interactions. The intensity of the peak in the scattered ion spectrum depends upon, in addition to the surface density of the scattering atom, the differential scattering cross section and the neutralization probability. The former has been generally calculated assuming a screened Coulomb potential, in a similar manner to HEIS. The neutralization probability is a more difficult problem, although the basic physical processes are known.³² The neutralization problem has been attacked in several ways; alkali metal beams,^{33,34} time-of-flight mass spectrometry,^{35,36} and neutral reionization.³⁷

The manner in which LEIS has been used to provide surface structural information falls into two main classes:

(1) simple experiments which yield crude, but often useful information. Thus the relative position of two atomic species in a surface, e.g., subsurface versus adsorbed, can sometimes be found by observing the ratio of their LEIS signals.

(2) More sophisticated studies where quantitative structural information is found from data obtained at several different incidence and exit angles. The surface unit cell can be directly imaged using multichannel plate detectors.³⁸

The latter types of investigations make use of the concept of the shadow cone and surface blocking as outlined earlier. If an atom falls within the shadow cone of another, then it cannot contribute to the scattered intensity. Thus, by measuring the scattered intensity from an adsorbate, for instance, at various azimuthal exit angles, the shadowing effect of substrate atoms can pinpoint the adsorbate location. For inert gas ions, the analysis is complicated by trajectory-dependent neutralization effects.³² While the use of alkali ions reduces the neutralization probability, multiple scattering effects often require comparisons with extensive Monte Carlo codes.^{39,40}

One of the most powerful applications of LEIS has been the development of impact collision ion scattering spectroscopy (ICISS).^{41,42} In this mode the scattering angle is set as close to 180° as possible. Accordingly, only ions having undergone head-on collisions (an impact parameter near to zero) are observed, reducing the effects of multiple scattering. At some critical incident polar angle, a sharp increase in the scattered intensity occurs. Each critical angle is geometrically related to the distance between the atoms in a particular row, and so, if the shape of the shadow cone is known, we can determine a number of interatomic distances by measurement of several critical angles. To avoid the use of a theoretical shadow cone, some workers have used expe mental cones previously measured on a surface of knov structure as a self-calibrating procedure.²⁹

Most LEIS experiments do not involve extensive coparisons of experimental data with calculations made f assumed surface structures, but rather derive structural formation from such experimental data as critical angles. a result R-factors do not seem to be in use in these type scattering studies.

In the low-energy regime, scattering from a welldered surface produces characteristic energy and angu distributions. As thermal vibrations act as a quasistatic s face disordering on the time-scale of the ion-surface intertion, they can have an influence on the spectra, and any rived structural results. Most authors have not attempted build in different Debye temperatures for surface atoms their interpretations, but there does appear to be an incre ing tendency for investigators to allow this as another str tural parameter to be fitted.^{43,44}

3. Evaluation Criteria

Determining a surface structure using ion scattering volves surface preparation, collection of the scattering da and derivation of the structure, possibly involving calcutions for a particular postulated surface structure and cc parison with the experimental data. Each of these stages associated with it certain problems that may affect the r ability of the result and may involve judgements that may open to more than one interpretation.

Hence a proper critical evaluation of a surface crysta graphic study involves a consideration of many different : tors, which may have complex interrelationships, that affect our confidence in the reported result.

The methodology for critically evaluating ion scat ing crystallographic data will focus principally on the n critical areas of the technique, the collection of data comparison of theory with experiment. Most workers h used tested and reliable computational schemes, hence exact method of calculation is not often a strong determir of reliability.

Given the many diverse components that go into a c plete study, and the many factors that can influence the ability of a given result, it is difficult to come up with se simple numerical index that would signify a "good" "bad" structure. The most realistic solution to providi confidence level for a given result is to draw up a lis criteria which would define a very reliable study. In s instances such a criterion might indeed be numerica contamination level in percent of a monolayer, or the n ber of datasets used in a comparison of theory and exp ment. In other instances we might be able to give a year answer to questions like "Is a reliability-factor used?" Sc times it may only be possible to reveal unquantifiable mis ings about some aspect of the procedures-for inst doubts as to a careful avoidance of disturbing effects suc beam damage.

Therefore, we will now examine each step of a ty_1 ion scattering experiment and discuss the factors that *a* the results. The criteria that are developed here form s for the columns reported in the main database table and ald be read before using the table for a proper underding of their meaning and function

3.1. Experimental Aspects

3.1.a. Surface Preparation

The preparation of the surface under study is such a lamental part of any surface crystallography experiment incumbent upon us to make a critical examination of the ribed procedures.

The first goal of any surface science experiment is to pare the surface under consideration in the required 1. The single-crystal sample is usually cut from a rod or e, oriented and polished using standard metallographic nods, and mounted on a manipulator. With care the orition of the polished crystal should be within 1°, or less, of desired plane. Few workers, however, explicitly state they check that the x-ray face, as found from a backction Laué photograph, is parallel to the polished optiace. This can be easily done using a small He–Ne alignt laser. As the metallographic techniques for preparing a hed crystal slice of a particular orientation are standard edures, we assume here that the sample is oriented to in 1°, unless the authors state otherwise.

The contamination and damage introduced during the ng and polishing processes is usually removed by cleanne surface to below some acceptable level of contaminausing thermal, chemical, or ion bombardment teches. Chemisorbed structures can then be obtained by ption. Analytical techniques such as Auger electron roscopy (AES)⁴⁵ or x-ray photoelectron spectroscopy 3)⁴⁶ can reveal adatom concentrations at the level of a percent of a monolayer coverage, and form useful adtechniques. Of course the ion scattering spectra themi, or surface nuclear reaction analysis (NRA)⁴⁷ can be to monitor surface composition, making the inclusion is other analytical techniques not strictly necessary.

The question of what constitutes a clean surface is of e a vexed one, and can depend very much on the sysind the requirements and sensitivity of the experiment. it is much more difficult to produce a truly clean iron mium surface, than a copper or gold surface. Or a sureconstruction might be turned on or inhibited by small nts of contamination. Nevertheless, we suggest the use (generous) figure of 5% of a monolayer to represent ber bound to an acceptable contamination level in ordiircumstances.

If necessity, LEED surface crystallography studies been carried out on well-defined highly ordered sur-Due to the local nature of the ion scattering process, striction disappears. However, many ion scattering s have been performed on systems that are known to ordered structures; in some cases this is merely asto be the case. It is most reassuring to know that the nental data is in fact from the same structure that nethods have studied. For this to be, some means has rovided to assess the surface order. The natural tool to LEED optics present in the sample chamber, to provide a qualitative check on the symmetry and order of the surface under examination. In the absence of any well-defined quantitative measure of surface crystallinity, workers generally rely on a visual judgement of a low background coupled with small, sharp diffraction spots to indicate a wellcrystallized surface.

Thus, in the area of surface preparation we can formulate a number of criteria for effective preparation:

(1) Is the contamination level below 5% of a monolayer? Are actual spectra shown, or peak ratios noted, to back-up this value?

(2) Are ancillary analytical methods used, and do they corroborate the ion scattering data?

(3) Is the surface highly crystalline? Are photographs of LEED patterns provided?

To be fully assured of adequate surface preparation we should be able to give an affirmative answer to all these questions. In fairness, however, it would be sufficient for an author to refer to a previous paper in which these details have been covered.

3.1.b. Data Collection and Surface Damage

Data collection in ion scattering can involve the measurement of a large number of scattering spectra taken at different incidence and scattering angles. Hence data collection times can be rather long and the question of surface damage becomes one of importance.

The number of surface atoms that are displaced or sputtered by an incident ion varies greatly with the substrate and the ion energy. High-energy ions, such as MeV protons, displace only about 10^{-3} substrate atoms per incident ion. This is a low rate of damage production; for a typical HEIS experimental beam dose of 10^{15} ions per cm², only $\sim 10^{12}$ atoms, or < 1% of a monolayer, are displaced in the near surface region. On the other hand, ions in the LEIS energy range can have sputtering yields greater than unity. In this case experiments must be performed at low dosages to avoid significant damage to the surface. It is certainly appropriate for authors, particularly at the lower ion energies, to quote the beam dose to which the sample was exposed.

It is particularly reassuring to find that closely similar sets of experimental data have been measured from more than one separately prepared sample. In general, however, we must acknowledge that preparing and cleaning are sufficiently difficult that such duplication of data may not be easy.

Based on the above arguments we can suggest the following criteria for effective data collection: (1) The beam dose should be reported, and should result in < 1% of a monolayer damage to the surface. (2) Ideally, identical data should have been obtained from more than one sample.

3.2. Structure Determination

The derivation of a surface structure from ion scattering data depends greatly upon the detail and precision desired in the final structure. It can be as simple as comparing the size of two spectral features, or as difficult as a multiparameter fit of much angular data with complex Monte Carlo calculations for many different assumed structures.

However, there are a number of considerations that apply to at least most experimental configurations and levels of sophistication. These concern the amount of data available, the procedure for comparing experiment and theory, and the difficulty of finding unique structural solutions. We suggest below a number of criteria in this area, and proceed to explain and justify them. These are: (1) At least two independent set of data should be available. (2) Where appropriate, a numerical reliability factor or index should be used. (3) Several surface structural models should be examined, possibly including changes in more than one interlayer spacing, registry shifts, and surface vibrational amplitudes. (4) Any estimated error should be consistent with the demonstrated procedures.

3.2.a. Amount of Experimental Data

One of the most noticeable aspects of the ion scattering literature are the variations in the amount and nature of the data collected in different studies. The effect is partly historical; many early studies fit a small amount of experimental data to find a surface structure, but as experimentalists have become more proficient, there is a tendency to collect more extensive datasets.

Obviously there exists a linkage between the total amount of data used and the reliance that we can place on the structural result. It is difficult to suggest any amount of data that represents an unacceptably small dataset; there appears to be little or no consensus on this point among practitioners. In the tables compiled in this review we have reported or made a best estimate, not always a trivial procedure in some cases, the number of incidence angles used, and the size of the total dataset. This latter quantity could be made up of a number of angular scans taken at different energies, or a number of azimuthal detection angles, or some combination. In some cases only "Many" suffices.

Despite the disclaimer announced above, it seems appropriate to at least attempt to define a minimum dataset size that would inspire confidence in the reader. We suggest that a minimum of two different experimental conditions, i.e., angle or energy combinations, should be measured.

3.2.b. Comparison of Theory and Experiment

In many cases the experimental data is compared with corresponding calculations to decide which model surface structure best fits the measured data. Many workers in the early days of the technique used visual methods of comparison. While the eye has excellent sensitivity for distinguishing small details between a pair of calculated and observed curves, it is very difficult to assess the cumulative fit of many such pairs and it can be hard to obtain agreement between different judges.

It is clearly desirable to have the work of comparing many sets of experimental and theoretical data done in an objective and consistent manner by computer. The lack of agreement between different workers as to what constitu a good reliability factor means that is difficult to find ma studies that use exactly the same index. Hence it is not usu ly possible to use R-factor values to distinguish between c fering results found by different groups. However, R-facto do have a very important role to play in finding an interna consistent best-fit structure for a particular set of experime tal data. The use of such quantitative measures does allo for a consistent evaluation of competing structural mod and of comparison of results from one laboratory to anoth

A problem that frequently arises in this context is the changes in a nonstructural parameter, particularly surfavibrational amplitudes, and changes in a structural quantisuch as a bond length, are coupled together. Thus, the valof the structural parameter producing the best fit betwee the observed and calculated data may change if the value the nonstructural parameter is altered. Hence it is importafor authors to state whether such effects have been inves gated.

We note here that it appears to be common in the i scattering literature for authors to suppress powers of ten presenting R-factor topographs. This can make comparis between studies carried out on different laboratories di cult.

Another difficulty is that of deciding when enough d ferent structural models have been tested to give us con dence that we are not resting in some local minimum of t parameter space, but are truly at the global minimum of t system. Once again, we cannot, in reality, assign any ha and fast numbers to this criterion. Its role will be essentially negative one; in cases where, for instance, only a very sm number of models were tested, it would have an impact in t total estimation of the reliability of the determination.

A final possible criterion refers to the error limits of their results quoted by some authors—thus a bond leng may be reported as being within 0.1 Å of a certain value. The value may result from the step used in the variation of structural parameter such as a layer spacing or bond lengt or may be derived from an interpolation of a grid of R-fact results. Here this criterion will again be used in a negati sense—that is, it will be noted if the quoted error does n appear to be consistent with the data and procedures d scribed in the paper.

3.3. Overall Assessment of Reliability

. Having enunciated several criteria for estimating t degree of confidence we find in a particular structure determination, it remains to try to find a way to wrap all the different factors into one overall assessment of the con dence level of the structure. As discussed earlier, this is ve difficult to do because of the varied nature of the differe criteria and the lack of a numerical basis for distinguishin conflicting results.

Accordingly, this critical compilation presents t reader with a rather complete picture of a study in a ve condensed form in Table 2. It is arranged so as to allow t reader to easily and quickly find a structure. Thus the read will quickly be able to tell to form a judgement as to t extent that a particular study has fulfilled the criteria su ested above. Table 2 is followed in Sec. 5 by an expanded iscussion with numerous figures and ancillary tables.

4. Surface Structure Compilations

4.1. Organization and Nomenclature

Table 2 presents the surface structure compilations. It ontains values of the pertinent experimental and theoretical arameters discussed earlier in a concise, but easily undertood form. Also the table shows structural and nonstruciral parameters derived from the experimental data. In adition, there are also short comments on interesting points of echnique, and simple descriptions of the derived structures iat cannot be easily shown numerically. As some structures re too complex to be easily summarized in this manner, iore detailed discussion can be found in Sec. 5.

The Table is organized so that a particular structure can e readily found. The entries are arranged with the following tiorities: (1) Alphabetically by substrate.

(2) Numerically by the surface plane Miller indices, ., (100) before (110) before (111).

(3) Alphabetically by adsorbate, when present.

(4) Size of the unit cell, i.e., (1×1) before (2×1) bere (2×2) . Here we arbitrarily assign $p(2 \times 2)$ higher priity than $c(2 \times 2)$.

(5) Chronologically by date of publication.

Below are listed explanations of some of the symbols ed as table headings and abbreviations and acronyms that ay be encountered in the body of the tables. When an entry ntains a dash (-), this indicates that this information was t specified. A query (?) indicates that the value of the rameter in question was discussed but not clearly defined. *bstrate (Subs.)*:

The chemical symbol of the substrate.

face (Surf.):

The Miller indices of the surface under investigation. *vorbate (Ads.)*:

The identity of any adsorbate present.

ucture (Struct.):

The symmetry of the surface structure present, using idard surface crystallographic notation.

erence (Ref.):

The reference number of the study as given in Section

hod (Meth.):

The type of ion scattering experiment performed. a Collection (Data Coll.):

The manner in which the data was collected. The acrois used are (see text for details):

CMA---cylindrical mirror (electrostatic) analyzer

ESA—electrostatic analyzer (sector, or toroidal)

ICISS-impact collision ion scattering spectroscopy

IAC---induced Auger channeling

LEIBAD—low-energy ion bombardment angular distions

LERS—low-energy recoil spectroscopy

MC---multichannel plates

NRECOIL—nuclear recoil spectrometry

SB—surface barrier detector

TOF-time-of-flight mass spectrometry

TC-transmission channeling

Ion:

The identity of the projectile ion(s).

Energy (E):

The ion energy in keV.

Dose:

The maximum ion dose seen by the area of the crystal under investigation in ions/ m^2 .

Contamination Level (Cont. level):

The reported level of surface contamination in monolayers, or other specified units. L(ow) indicates an unspecified "clean" state.

Other Techniques (Other tech):

Other techniques that were used during the investigation to monitor, e.g, surface composition (AES, XPS, etc.) or surface structure (LEED). Acronyms used here are:

AES—Auger electron spectroscopy.

LEED-low-energy electron diffraction

MEED-medium-energy electron diffraction

NRA—nuclear reaction analysis

PIXE—proton-induced x-ray emission

RBS-Rutherford backscattering spectroscopy.

UPS-ultraviolet photoelectron spectroscopy

WF-work function

XPS-x-ray photoelectron spectroscopy

XRD-x-ray diffraction

When spectra are reproduced then S appears in parentheses. Number of Angles (Angs.):

The number of angles of incidence at which data was taken.

Data Sets (Data):

The total number of datasets measured (all angles and energies—see text).

Temperature (Temp. (K)):

The temperature at which the experiment was performed in degrees K.

Calculation (Calcs.):

The method of calculation used; by reference.

R-factor (R-):

Only the type of R-factor is quoted because of doubts over suppressed powers of ten. For R-factor definitions, see Sec. 2.2.

Debye (K):

The value of the surface Debye temperature (in K) used in calculations. In some cases the parallel (\parallel) and perpendicular (1) components are given separately. *d-B*:

The value of the interlayer spacing in the bulk material in Å.

d-0:

The value of the distance of an overlayer from the center of the topmost layer substrate in the normal direction (Å). Error in parentheses when given. In parentheses is given the adsorption site symmetry as below. (see Scc. 5.2 for more detail)

 $4\mathbf{F} = 4$ -fold coordinate site, e.g., FCC(100)

3F = 3-fold coordinate site, e.g., FCC(111)

| | | | | | | Data | | | Dote | Cont. | Other | | | Temp. | | | Debye | d-B | d-C | <i>d-</i> 1 | d-2 | |
|------------|-------|------|----------------|------|-------|------------|------|------------|---------------------------|-------|----------------|-------|------|---------|--------|-----|-------|-------|------------|-------------|------------|--|
| S . | Surf. | Ads. | Struct. | Ref. | Meth | . coll. | Ion | E(keV) | (<i>m</i> ²) | level | tech. | Angs. | Data | (K) | Cales. | R | (K) | (Å) | (Ä) | (%) | (%) | Comments |
| | 110 | | (1×1) | 17 | HEIS | SB | He | 400 | | L | LEED/AES | 3 | 3 | 300 | 7 | RIS | 149 | 1.445 | | - 78(2.5) | + 4.3(25) | |
| | 110 | _ | (1×1) | 25 | MEI | 5 ESA/MC | н | 53.98 | ? | L | LEED/AES | 3 | 4 | 300 | 2 | Riv | 150 | 1.445 | - | - 9.5(2.0) | + 6.0(2.5) | _ |
| | 110 | 0 | (2×1) | 48 | LEIS | ESA | He | 06 | | L(S) | LEED/AES | 2 | 2 | | 48 | | _ | 1.445 | 0.0 (2F-L) | _ | | O in surface channels in bridge site, |
| | | | | | | | | | | | | | | | | | | | | | | close to coplanar with top layer Ag atoms. |
| | 111 | Au | | 49 | HEIS | SB | He | 1000 | | L | LEED/AES | 2 | 4 | 300 | | _ | _ | 2.359 | | - | - | Closely epitaxial layer by layer growth. |
| | | | | | | | | | | | | | | | | | | | | | | Au mainly (90%) in FCC sites. |
| | . 110 | - | (1×2) | 16 | HEIS | SB | He | 200-1600 | ? | L | LEED/AES | 2 | 4 | 100,293 | 11 | RSQ | 110 | 1.442 | _ | + / - 17 | | Confirm missing-row model with lateral |
| | | | | | | | | | | | | | | | | | | | | | | displacements in 2nd layer 0.12 Å (100 K), |
| | | | | | | | | | | | | | | | | | | | | | | 0.18 Å (298 K). |
| | 110 | | () | 60 | uri | 60 | u. | | | | VPD | , | , | 100 | 7 | | | 1 447 | | _ | | Missing-row structure with lateral pairing |
| | 110 | | (1×2) | 50 | пы | 55 | П¢ | | | | AND . | 4 | 2 | 100 | , | | | 1.442 | | | | in 2nd row of 0.12 Å possibly outward |
| | | | | | | | | | | | | | | | | | | | | | | manufow of 0.12 At possibly butward |
| | | | | | | | | | | | | | | 200 | | | | | | | | relaxation. |
| | 110 | - | (1×2) | 51 | LEIS | ESA | K.He | G 6 | - | L | | 2 | 2 | 300 | 53 | | | 1.442 | - | - | - | Data does not support (1) distorted |
| | | | | | | | | | | | | | | | | | | | | | | hexagonal overlayer, (ii) unrelaxed |
| | | | | | | | | | | | | | | | | | | | | | | missing-row or (iii) high degree of |
| | | | | | | | | | | | | | | | | | | | | | | disorder |
| | 110 | | (1×2) | 52 | MEI | S SB | He | 300 | - | L | LEED/AES | 2 | 2 | | 9 | | | 1.442 | - | | | Data agree best with large expansion model |
| | | | | | | | | | | | | | | | | | | | | | | [54], or small contraction and 2nd layer |
| | | | | | | | | | | | | | | | | | | | | | | expansion [55]. Could not match line widths. |
| | 110 | | (1×2) | 56 | MEI | S ESA/MC | н | 65,200 | _ | | LEED | 3 | 3 | | 2,7 | _ | 130 | 1.442 | - | - 18 | +4 | Three samples. Confirm missing-row structure |
| | | | | | | | | | | | | | | | | | | | | | | with 3rd layer buckling. Difficult to dis- |
| | | | | | | | | | | | | | | | | | | | | | | tinguish pairing effects in 2nd layer |
| | | | | | | | | | | | | | | | | | | | | | | from vibrational effects. |
| | 110 | | (1×2) | 57 | LEIS | ESA/TOF | Ne.N | a 2 | ? | L | LEED | 1 | 4 + | 300-800 | 57 | | _ | 1.442 | | - 13.9(4.8) | | Extension of [57]. Took data at several |
| | | | (1/(-/ | | | | | | | | | | | | | | | | | | | temperatures. Favor missing-row structure |
| | | | | | | | | | | | | | | | | | | | | | | with contraction. Followed phase transition |
| | | | | | | | | | | | | | | | | | | | | | | to (1×1) |
| | 110 | | (1)(2) | 50 | I EIS | LOISE /TOF | No | | 0 | | | 6 | 6 | | | | | 1 442 | | 0.4(6.9) | | A greek with missing-row model |
| | 110 | | (1 × 2) | 36 | LEIS | IC135/ TOP | 140 | • | : | _ | | 2 | | | | | | 1.442 | - | - 0.4(0.7) | - | Agrees with massing-row model. |
| | . 110 | - | (1×2) | 59 | LEIS | - | ĸ | 0.6 | - | | | 2 | 2 | | 55 | _ | | 1.442 | | - 1.3(2.7) | | Use data from [55]. Lateral parting dis- |
| | | | | | | | | | | _ | | _ | _ | | | | | | | | | placement in 2nd layer < 0.10 A. |
| | 110 | | (1×2) | 60 | MEI | S ESA/MC | н | 65,180 | - | L | LEED | 2 | 2 | | | _ | - | 1.442 | - | - 8 | _ | Missing-row structure. |
|) | 111 | | p(2×1) | 61 | MEI | S ESA | н | 49 | 6E+21 | | LEED | 2 | 5 | 300 | 2 | R2v | | 0.515 | | - | - | Formed after 950 °C anneal. Data compatible |
| | | | | | | | | | | | | | | | | | | | | | | with pi-bonded chain model with dimeriza- |
| | | | | | | | | | | | | | | | | | | | | | | tion parallel to chains [62]. |
|) | 111 | н | (1×1) | 61 | MEI | 5 ESA | н | . 19 | 6E+21 | _ | LEED | 2 | 5 | 300 | 2 | R2v | _ | 0.515 | | < 10 | - | H-saturated surface. Small relaxation |
| | | | | | | | | | | | | | | | | | | | | | | agrees with LEED [63]. |
| | 111 | | | 153 | HEIS | - | He | 3500 | 6E+19 | L | | 2 | 2 | | | | | _ | | _ | - | Film grown by MBE on Si(111) |
| | | | | | | | | | | | | | | • | | | | | | | | at 700 °C. Films less than |
| | | | | | | | | | | | | | | | | | | | | | | 200 nm thick were strained. |
| | 100 | A | 0(7×7) | 64 | 1 519 | СМА | LL. | | 2 | | LEED/AES/UPS | 1 | 1 | | | | _ | 1 807 | | | | Ordered surface resembles Cu3Au(100) |
| | 100 | Au | u(2×2) | 04 | LEIS | CMA | rie | | • | L | 222D/ AC3/ 013 | | • | | | | - | 1.007 | | | _ | 50% Au in the laver |
| | | | | | | | | | | | | | | | | | | | | | / | 55 / Au ni top layer. |
| | 100 | 0 | c(2×2) | 32 | LEIS | CMA | He | 1 | - | L | LEED/AES | 2 | 2 | 625 | 32 | | | 1.807 | - | - | | Needed to include ion-atom neutralization. |
| | | | | | | | | ÷ | | | | | | | | | | | | | | Difficult to distinguish 2F bridge from 4F |
| | | | | | | | | | | | | | | | | | | | | | | hollow adsorption sites. |
| | 100 | 0 | e(2×2) | 65 | LEIS | ESA | Ne | + | - | | | Many | Many | | | | | 1.807 | - | - | | No reconstruction; 2 sites involved, |
| | | | | | | | | | | | | | | | | | | | | | | possibly 2F/4F. At higher coverages |
| | | | | | | | | | | | | | | | | | | | | | | (12×212)R45 structure involves O pene- |

tenting caluadaa

| <i>v</i> i | | | | | | | | | | | | | | • • | | | | | | | | |
|------------|--------------------|--------|------|---------|------|--------------|----------------------|----------|---------------------------|----------|--------------|-------|------|---------|-------|----------------|---------|-------|---------------------|------------|-----------|---|
| ç | Subs. | Surf. | Ads. | Struct. | Ref. | Meth. coll. | lon | E(keV) | (<i>m</i> ²) | level | tech. | Angs. | Data | (K) | Calcs | . R | (K) | (Å) | (Å) | (%) | (%) | Comments |
| em. | Cu | 110 | | (1×1) | 66 | HEIS SB | He | 300 | 6E + 19 | L | LEED/AES | 2 | 2 | 300 | 11 | RWIS | 250 | 1.278 | _ | - 5.3 | + 3.3 | Agrees with LEED [66b]. |
| P | Cu | 110 | | (1×1) | 67 | LEIS ICISS | Li | 5 | ? | L | LEED/AES | 3 | 3 | 300 | 68 | | 258 | 1.278 | | - 10(5) | - | |
| <u>.</u> | Cu | 110 | | (1×1) | 69 | MEIS ESA/MC | н ′ | 100 | 4E + 20 | L | LEED/AES | 2 | 2 | 323 | 11 | RWIS | 205 | 1.278 | | - 7.5(1.5) | +2.5(1.5) | - |
| 0 | Cu | 110 | о | (2×1) | 70 | LEIS NRECOIL | Ne, H ₂ O | 4 | ? | Ľ | LEED | 4 | 8 | | _ | . . | | 1.278 | (2F – L) | - | | 0 atoms in bridge sites as before but |
| ត | | | | | | | | | | | | | | | | | | | | | | Cu atoms in missing-row reconstruction. |
| < | Си | 110 | 0 | (2×1) | 71 | HEIS SB | He | 200-2000 | - | L | LEED/AES | 2 | 10 | 300 | н | RWIS | 250 | 1.278 | _ | See Notes | - | No agreement with missing-row model. |
| <u>e</u> . | | | | | | | | | | | | | | | | | | | | | | Best agreement with buckled surface model * |
| 19 | | | | | | | | | | | | | | | | | | | | | | with every 2nd [001] row displaced out by |
| z | | | | | | | | | | | | | | | | | | | | | | 0.27(05) Å, whole 2nd layer shifts out by |
| ō | | | | | | | | | | | | | | | | | | | | | | 0.06(03) Å. Adsorption at 100 K. |
| | Cu | 110 | 0 | (2×1) | 67 | LEIS ICISS | Li | 5 | ? | Ĺ | LEED/AES | 3 | 3 | 300 | 68 | | 258 | 1.278 | | + 25 | - 10 | 200L O /100 °C for 5 min. Data consistent |
| ig i | | | | | | | | | | | | | | | | | | | | | | with missing, but not buckled-row, |
| ő | | | | | | | | | | | | | | | | | | | | | | reconstruction. |
| | Cu | 110 | 0 | | 72 | LEIS ESA | Ne | 3-5 | — | - | Many | Many | Many | y | 10 | against . | | 1.278 | $-0.\epsilon(2F-L)$ | | <u> </u> | Little evidence for reconstruction, |
| | | | | | | | | | | | | | | | | | | | | | | 0 in long bridge site. |
| | Cu | 110 | 0 | - | 29 | LEIS ICISS | Na | 2 | - | L | LEED/AES/WF | 5 | 5 | | | | | 1.278 | — | | | 10-5 mbar/s O_2 at room temp. and anneal |
| | | | | | | | | | | | | | | | | | | | | | | 370 °C min. Favor missing row model. |
| | Cu | 111 | 0 | | 73 | LEIS ICISS | He | 2 | · | L | LEED/AES/WF | 3 | 3 | 300 | | _ | _ | 2.087 | | _ | _ | Surface reconstructed with Cu atoms dis- |
| | | | | | | | | | | | | | | | | | | | | | | placed by 0.3 Å. No subsurface O. |
| | Cu | 410 | | (1×1) | 74 | LEIS ESA | Ar,Ne | 8-11 | ? | | | 4 | 8 | 540 | 74 | _ | | | | _ | | Showed terraces 4 atoms wide separated |
| | | | | | | | | | | | | | | | | | | | | | | by 1-atom steps. |
| | Cu | 410 | 0 | - | 75 | LEIS ESA | Ne,Na | 5 | ? | - | | 2 | 3 | | 75 | - | 147 | | | | | 0 at hollow sites of step edges. |
| | Cu | 16,1,1 | | (1×1) | 76 | MEIS SB | He | Several | ? | C,0<3% | LEED/AES/NRA | Many | Man | y 300 | 76 | | 350 | | _ | - 3* | - | *in (100) direction. No step-edge re- |
| | | | | | | | | | | | | | | | | | · | | | | | laxation. O adsorption reverses sign of |
| | | | | | | | | | | | | | | | | | | | | | | Cu relaxation and induces facetting. |
| | Cu _s Au | 100 | | (1×1) | 77 | LEIS TOF | Ne | 5,9.5 | - | | LEED/AES | 2 | 3 | Several | - | _ | _ | | - | _ | - | 50% Au in top layer; 0% in 2nd. |
| | Fe | 100 | _ | (1×1) | 78 | LEIS TOF | Ne | 9.5 | | Some C,N | LEED/AES | 3 | Man | y 300 | 10 | | | 1.433 | 0 | | | 4% Sn/Fe alloy stoichiometry retained if |
| | | | | | | | | | | | | | | | | | | | | | | sputter <400 °C. No reconstruction. |
| | Fe | 100 | 0 | (1×1) | 79 | LEIS ESA/TOF | Ne | 5 | | L | - | 2 | 2 | 300 | 10 | | | 1.433 | 0.56()5)(4F) | | - | 15L O2/room temp than anneal at 700 K/15 |
| | | | | | | | | | | | | | | | | | | | | | | min. gave ordered 1ML coverage. |
| | Fe | 100 | Sn | (2×2) | 80 | LEIS TOF | Ne | 9.5 | - | | LEED/AES | 2 | 4 | 300 | 40 | | - | 1.433 | | | - | Segregated from 1.7% Sn-Fe alloy by |
| | | | | | | | | | | | | | | | | | | | | | | heating 600 °C/1 hr. Top layer all |
| | | | | | | | | | | | | | | | | | | | | | | Sn in Fe sites, 2nd layer all Fe. |
| | | | | | | | | | | | | | | | | | | | | | | New LEED (2×2) may be due to |
| | | | | | | | | | | | | | | | | | | | | | | adsorbed Sn. |
| | GaAs | 100 | _ | c(4×4) | 81 | HEIS SB | He | 2000 | 1.5E + 20 | _ | LEED/PIXE | _ | _ | | 9,11 | - | 333,291 | 1.414 | _ | | _ | Grown by MBE. Significant lateral dis- |
| | | | | | | | | | • | | | | | | | | | | | | | placements of 1st layer As and sub- |
| | | | | | | | | | | | | | | | | | | | | | | surface strain. |
| | GaAs | 100 | н | (1×1) | 81 | HEIS SB | He | 2000 | 1.5E + 20 | | LEED/PIXE | _ | | | 9,11 | | 333,291 | 1.414 | _ | | | H2/hot filament; surface is bulklike. |
| | GaAs | 110 | _ | (1×1) | 82a | HEIS SB | He | 2000 | 1.5E + 20 | L | LEED/AES | 2 | 2 | | 9,11 | | 333,291 | 1.999 | | _ | | Annealed 630 °C. Ga, As have small lat- |
| | | | | | | | | | | | | | | | | | | | | | | eral displacements; data consistent with |
| | | | | | | | | | | | | | | | | | | | | | | relaxed-bond, 7* Ga-As chain rotation |
| | | | | | | | | | | | | | | | | | | | | | | model. |
| | GaAs | 110 | - | (1×1) | 83 | MEIS ESA | н | 50,100 | 1E + 20 | L | LEED | 2 | 4 | 300 | 84 | R27 | | 1.999 | | | - | Ga-As chains rotate through 29°, con- |
| | | | | | | | | | | | | | | | | | | | | | | serving bond lengths. Attribute dis- |
| | | | | | | | | | | | | | | | | | | | | | | agreement with [82a] to high anneal- |
| | | | | | | | | | | | | | | | | | | | | | | ing temperature. |
| | | | | | | | | | | | | | | | | | | | | | | |

| | | | | | Data | | | Dose : | Conl. | Other | | | Temp. | | | Debve | d-B | d-0 | d-1 | d-2 | |
|-------|--------|-------|---------|-------------|--------------|-------|--------|------------|-------|--------------|-------|------|-------|--------|------|------------|--------|--------------|------------|------------|---|
| Subs. | Surf. | Ads. | Struct. | Ref. | Meth. coli. | Ion | E(keV) | (m^{-2}) | level | tech. | Angs. | Data | (K) | Cales. | R | (K) | (Å) | (Å) | (%) | (%) | Comments |
| ~ | | | | | | | | | | | | | | | | | | | | | |
| GaA | \$ 110 | Au,Pd | (1×1) | ξ2р | HEIS SB | He | 2000 | 1.5E + 20 | L | MEED/AES | 2 | 2 | 300 | 9,12 | - 1 | 333,291 | 1.999 | - | - | •••• | Pd, but not Au, affects substrate struc- ture substantially. |
| GaSt | 110 | | (1×1) | 15Ъ | MEIS ESA/MC | He | 174 | 6E + 18 | L | - | 1 | 1 | 300 | 2 | R2v | 222,136 | 2.163 | - | See Notes | - | Bond lengths conserved, Ga-Sb bond rotated by 29°. Thermal vibrational amplitudes of surface atoms increased by a |
| | | | | | | | | | | | | | | | | | | | | | factor of 1.5. |
| InAs | 110 | | (1×1) | 15a | MEIS ESA/MC | He | 174 | 6E + 18 | L, | - | 1 | 1 | 300 | 2 | R2v | | 2.142 | - | See Notes | | Similar structure to GaAs and GaSb with with 30° rotation. |
| Ir | 110 | | (1×2) | 40 | MEIS ESA/MC | н | 65,180 | | L | LEED | 1 | 1 | | | - | | 1.352 | - | - 10 | - | Missing-row structure. |
| LaB | 100 | - | (1×1) | ł6 | LEIS ESA | He | 1 | | L | LEED/XPS | I | 1 | | | - | - | - | anna . | - | | Surface terminated by La; in case of SmB ₆ Coverage by Sr1 less complete. |
| LaB | 111 | - | (1×1) | \$7 | LEIS ESA | He | 1 | - | L | LEED/XPS/UPS | 3 | 3 | 300 | ~~ | | _ | 1.20 | - | - | | La atoms at surface may be relaxed outwards. |
| Mo | 111 | | (1×1) | 18 | LEIS ESA | Li | 1 | ? | Sm.C | LEED/AES | 10 | 10 | 300 | 40 | - | _ | 0.907 | | - 18(2) | + 4(4) | |
| Ni | 100 | - | (1×1) | 19 | MEIS ESA/SB | н | 52.98 | 1E + 19 | 1. | LEED/AES | 2 | 3 | 370 | 40 | _ | 285 | 1.762 | _ | - 3.2 | + 1 | Surface Debye temperature significantly |
| | 100 | | (1)(1) | ., | | | | | 2 | | - | | 5.0 | 10 | | 205 | | | | , . | increased relative to bulk. |
| Ni | 100 | D | | 90 | HEIS TC | He | 800 | ? | L | LEED/AES/RBS | 3 | 3 | 120 | 91 | - | 375 | 1.762 | 0.5(0.1)(4F) | | | Grown epitaxially on NaCl(100) and |
| | | | | | | | | | | | | | | | | | | | | | floated onto Nisupport. Used |
| | | | | | | | | | | | | | | | | | | | | | NRA to detect D. |
| Ni | 100 | 0 | (2×1) | 100 | LEIS ESA | Ar,Ne | 6 | - | | 3 | 4 | 12 | 300 | - | | - | 1.246< | (0.5(2F-L) | - | | Missing-row model favored; O in long- |
| | | | | | | | | | | | | | | | | | | | | | bridge sites. |
| Ni | 100 | 0 | c(2×2) | 92 | LEIS — | He | 1 | | L | LEED | 1 | 1 | 300 | _ | - | | 1.762 | 0.9(0.2) | | | O in 4F hollow site. |
| Ni | 100 | 0 | c(2×2) | \$ 9 | MEIS ESA/SB | н | 52,98 | 1E + 19 | L | LEED/AES | 2 | 2 | 370 | 89 | - | 285 | 1.762 | 0.86(4F) | + 5.2 | - | - |
| Ní | 100 | s | c(2×2) | 43 | LEIS ICISS | Ne | 5 | 6E + 18 | - | LEED | 2 | 2 | - | - | | | 1.762 | 1.40(0.05) | ~ | | |
| Ni | 100 | Te | c(2×2) | 90a | HEIS TC | He | 2000 | | L | LEED/AES/RBS | 2 | 2 | 170 | 91 | | 375 | 1.762 | 1.9(0.1)(4F) | | | Grown on NaCl(100). Te in 4F hollow sites. |
| Ni | 110 | ~ | (1×1) | 94 | MEIS ESA | н | 160200 | | L | | 2 | 2 | 300 | - | | | 1.246 | - | 0 | | - |
| Ni | 110 | - | (1×1) | \$5 | MEIS ESA | н | 100 | 3E + 20 | L | - | 1 | 1 | 300 | - | | · <u>-</u> | 1.246 | - | - 4(1) | | With $0.33ML 0, d-1 is + 1(1).$ |
| Ni | 110 | - | (1×1) | •6 | HEIS SB | He | 300 | ? | L | LEED/AES | 2 | 2 | 298 | 11 | RWIS | 325 | 1.246 | | - 4.8(1.7) | + 2.4(1.2) | |
| Ni | 110 | | (1×1) | \$7 | MEIS SB | н | 100 | ? | L | LEED/AES | 2 | 2 | - | | - | — | 1.246 | _ | - 4(1) | | |
| Ni | 110 | | (1×1) | 98 | MEIS ESA/SB | н | 110 | ? | L | LEED/AES | 3 | 3 | 300 | 9,12 | RWIS | 395 | 1.246 | - | - 9.0(1.0) | + 3.5(1.5) | Previous discrepancies with LEED |
| | | | | | | | | | | | | | | | | | | | | | attributed to chanliness problems. |
| Ni | 110 | C,O | - | 19 | HEIS SB | D | 1200 | ~ | - | | 2 | 2 | 300 | - | | - | 1.246 | (2F-L) | | | O and C in lonz-bridge positions. |
| | | | | | | | | | | | | | | | | | | | | | Identified by nuclear reactions. |
| Ni | 110 | 0 | (2×1) | 101 | MEIS ESA/MC | н | 100 | 2E + 19 | L | LEED/AES | 2 | 2 | 370 | 22 | | | 1.246 | _ | | | 3 min at 1×10-9 Torr oxygen for best |
| | | | | | | | | | | | | | | | | | | | | | LEED pattern. Estimate that ~ 50% |
| | | | | | | | | | | | | | | | | | | | | | of surface covered by missing-row O-induced |
| | | | | | | | | | | | | | | | | | | | | | reconstruction. |
| Ni | 110 | 0 | (2×1) | 102 | MEIS IAC | н | 150 | 1E + 19 | L | | 3 | 3 | 300 | ? | | 260 | 1.246 | 2.5(1.5) | - | | 2L O2 at 350 K for 0.5ML. Prefer saw- |
| | | | | | | | | | | | | | | | | | | | / | | tooth rather than missing-row model. O atoms |
| | | | | | | | | | | | | | | | | | | | | | in long-bridge site. |
| Ni | 110 | 0 | (2×1) | 103 | LEIS ICISS | Na | 2 | 1E + 17 | L | LEED/AES | 3 | 3 | | - | ~~ | - | 1.246 | 0.25(2F-L) | | | Missing-row structure; O in (001) |
| | | | | | | | | | | | | | | | | | | | | | bridge site. |
| Ni | 110 | о | (2×1) | 104 | LEIS NRECOIL | Ne | 2 | ? | L | _ | 4 | 4 | < 350 | - | | | 1.246 | 0.23(2F-L) | ~ | | O in long-bridge site in (001) direction. |

TABLE 2. Surface structures determined by ion scattering (continued).

| | | | | Data | | | Dose | Cont. | Other | | Temp. | | Debye | 1-B d-O | <i>d</i> -1 | <i>d</i> -2 | |
|------------------------|---------|------|-------|-----------|-------|-----------|-------------------|--------------|----------|---------|-----------|--------|--------------------------------|--------------------|--------------|---------------|--|
| iubs. Surf. Ads. | Struct. | Ref. | Meth. | coll. | lon | E(keV) | (m ²) | level | tech. | Angs. D | ata (K) | Cales. | ₹ (K) | (Ă) (Ă) | (%) | (%) | Comments |
| √i 110 S | c(2×2) | 105 | MEIS | ESA | н | 100 | 2E + 20 | L | _ | I | 1 298 | | | 1.246 0.87(03)(4F) | + 6 | | Structure assumed for 0.5ML S. Bond length Ni-S 2.32A. |
| ∛i 110 S | c(2×2) | 93 | LEIS | ICISS | Ne | 5 | 6E + 18 | - | LEED | 3 | 3 — | | | 1.246 0.89(0.05) | | - | Possible substrate rearrangement. |
| Ni 111 — | (1×1) | 106 | HEIS | SB | He | 500-2000 | 6E + 18 | 0.1% | MEED/AES | 1 | 1 300 | 9 | - 330 | 2.035 | < 1 | | _ |
| Ni 111 CO | (2×2) | 107 | LEIS | ESA | He | 1.4 | _ | | LEED/AES | 4 | 4 | | | 2.035 | _ | | CO associatively bonded through C atom: |
| | | | | | | | | | | | | | | | | | could not decide site. Same result |
| | | | | | | | | | | | | | | ~ | | | for lower coverage $(\sqrt{7/2} \times \sqrt{7/2})$ R19.1 |
| | | | | | | | | | | | | | | | | | structure. |
| Ni 111 O | p(2×2) | 108 | HEIS | · | He | 500-2000 | _ | L | LEED/AES | 2 | 2 298 | 9,11 | | 2.035 — | + 7.4 | _ | Adsorbate-induced expansion also seen for $(\sqrt{3} \times \sqrt{3})$ R 30 structure |
| li 111 O | p(2×2) | 106 | HEIS | - | He | 500-2000 | - | 0.1% | MEED/AES | 2 | 2 300 | 9 | | 2.035 | + 7.3 | - | |
| ii 111 S | (2×2) | 93 | LEIS | ICISS | Ne | 5 | 6E + 18 | | LEED | 3 | 3 — | - | | 2.035 1.61(0.06) | | _ | - |
| äAl 110 — | (1×1) | 109 | MEIS | SB | Н | 100 | | L | LEED | 2 | 2 | 53 | RIS 220,320 | 2.04 — | - 7Ni, + 5Ai | + 1Ni, - 1Al | 10% first layer ripple, Al on top. |
| liSi, 100 — | (1×1) | 110 | LEIS | LEIBAD | Li.He | 5 | 3E + 19 | L | LEED/AES | 2 | 6+ | 111 | | 1.351 — | - 22(4) | - | 90Å film on Si(100). LEED 1(V) curves agreed with [112]. Bulk-like Si termination; 25–30% vacancies. |
| ъ 110 — | (1×1) | 113 | HEIS | EAS/MC | н | 50,97 | | L | LEED/AES | 1 | 2 300 | 2,9 | R2v 65 | 1.75 — | 15.9(2.5) | + 7.9 | _ |
| 1 110 H | (1×2) | 114 | LEIS | ICISS/TOF | Ne | 2 | _ | L | LEED | 5 | 5 120 | | | 1.372 — | | . | Row-pairing model preferred. Alternat- |
| | | | | | | | | | | | | | | | | | ing lateral displacements of every |
| | | | | | | | | | | | | | | ÷ | | | other (110) row of about 0.4 Å with |
| | | | | | | | | | | | | | | | | | the same vertical shift. |
| d 111 — | (1×1) | 115 | HEIS | SB | He | 1800 | | L | LEED/AES | 3 | 5 300 | - | | 2.240 — | 0 | - | No relaxation. |
| d 111 Au | (1×1) | 115 | HEIS | SB | He | 1800 | - | L | LEED/AES | 3 | 5 300 | - | | 2.240 | - | | Au grows pseudomorphically until 2 Ä thic |
| | | | | | | | | | | | | | | | | | then transition to strained |
| | | | | | | | | | | | | | | | | | misfit state. |
| t 100 H | (5×20) | 116 | HEIS | SB | He | 1000-2000 | ? | L | LEED/NRA | 2 | 4 120,297 | 118 | - 239 | 1.961 — | 0(0.5) | | Reconstruction involves lateral diplace- |
| | | | | | | | | | | | | | | | | | of complete rows of atoms. |
| 100 H ₂ ,CO | (5×20) | 117 | HEIS | SB | He | 2000 | ? | L | LEED/XPS | 2 | 4 175 | 118 | - 115 | 1.961 — | < 1 | _ | Same result for both adsorbates. |
| 110 | (1×2) | 119 | LEIS | ICISS | Na | 2 | 1E + 17 | L | LEED/AES | 7 | 7 — | | | 1.387 | - | | Missing-row structure pref- |
| | | | | | | | | | | | | | | | 24 | | ferred, but some disorder. |
| i 111 | (1×1) | 121 | HEIS | SB | He | 400 | | < 0. IML | LEED/AES | 1 | 1 300 | ? | — See Note | s 2.264 — | < 2 40 | _ | Used Debye temperatures of 115 K perpen- |
| | | | | | | | | | | | | | | | | | dicular and 235 K parallel. |
| t iii — | (1×1) | 122 | HEIS | 58 | не | 2000 | See Notes | < 0.1ML | _ | 3 | 6 40-300 | . 123 | - 200-400 | 2.204 | + 1.3(0.4) | _ | fer earlier results showing large |
| | | | | | | | | | | | | | | | | | relevation (124) |
| | (1×1) | 125 | MEIS | ESA | U | 172 | | -0 IMI | | | , | | - Dulk | 3 364 | 15(10) | | relaxation (124). |
| 997 H | | 126 | LEIS | LERSTOF | Ne | 10 | _ | I I | _ | | 2 220 | _ | 174 | -0.7(0.2)(3F) | + 1.5(1.0) | | Also measured for Pt(445) surface |
| | | 120 | 2010 | EEKO, TOT | | | | 5 | | • | 2 220 | | | 0.17(0.27(517) | | | H occupies 3F hollow FCC site |
| | | | | | | | | | | | | | | | | | regardless of step orientation. |
| 100 (H) | (2×1) | 127 | HEIS | SB | He | 100-2000 | - | C/Si < 0.002 | LEED/AES | 1 M | lany 300 | _ | | 1.358 — | | | Compared with (1×1)-H termination. |
| | | | | | | | | | | | | | | | | | Evidence for subsurface strain with atomic |
| | | | | | | | | | | | | | | | | | displacements > 0.15 Å for at least 3 layers |
| 100 — | (2×1) | 41 | LEIS | ICISS | He | 1 | | L | LEED | 2 | 2 | _ | | 1.358 | _ ` | _ | Surface dimers; intradimer distance |
| | | | | | | | | | | | | | | | | | parallel to surface of 2.4(0.1) Å. |
| | | | | | | | | | | | | | | | | | Agrees with buckled dimer model [131]. |

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| TABLE 2. Surface structures determined by ion scatt | tering | (continued). |
|---|--------|--------------|
|---|--------|--------------|

| | | | | | Data | | | Dose | Cont. | Other | | | Temp. | | | Debye | d-B | d-0 | d-1 | d-2 | |
|------------|-------------|---------------------|------|-------|--------|-------------|-----------|---------------------------|--------------|----------|-------|------|-------|--------|-----|-----------|-------|-------------------------|-----------|-----|--|
| ubs. Surf. | Ads. | Struct. | Ref. | Meth. | coll. | lon | E(keV) | (<i>m</i> ²) | level | tech. | Angs. | Data | (K) | Cales. | R | (K) | (Å) | (Å) | (%) | (%) | Comments |
| i 100 | | (2×1) | 128 | MEIS | ESA | н | 50-150 | SE + 19 | LC,O | LEED/AES | 3 | 7 | 320 | 22 | | See Notes | 1.358 | · | | _ | Agreement best with buckled dimer model [131]. Parallel |
| | | | | | | | | | | | | | | | | | | | | | shifts of > 0.5 Å and subsurface distortions |
| | | | | | | | | | | | | | | | | | | | | | up to 3 layers deep. See also [129b]. |
| i 100 | | (2×1) | 130 | HEIS | TR/SB | He | 1000,2000 | _ | L | MEED/AES | 2 | 3 | _ | 9 | | 670(B) | 1.358 | No. of Concession, Name | | _ | YJM model [132] showed better agreement than |
| | | | | | | | | | | | | | | | | | | | | | symmetric [133] or buckled dimers |
| | | | | | | | | | | | | | | | | | | | | | [131] models. |
| i 100 | Au | | 134 | HEIS | тс | He | 2000 | ? | L | MEED/AES | 1 | Many | 300 | | | - | 1.358 | | | - | Si(100) film made by selective etching. Initial |
| | | | | | | | | | | | | | | | | | | | | | Au partially registered more random as |
| | | | | | | | | | | | | | | | | | | | | | approach 1 ML. Intermixing at 4 ML. |
| i 100 | н | $(1 \times 1) - 2H$ | 129 | MEIS | ESA | Е | 50-100 | - | C/Si < 0.002 | LEED/AES | 2 | 5 | 323 | 11,22 | - | 230 | 1.358 | - | - 6(3) | | 3000L H ₂ with hot filament from (2×1) |
| | | | | | | | | | | | | | | | | | | | | | clean Si(100). |
| 100 | Pd | (2×1) | 159 | MEIS | ESA | Fe | 98,174 | - | < 0.3% | LEED/EAS | 1 | 1 | - | | | _ · | 1,358 | | | - | Mixing occurs < 1 ML. Above 1 ML forms Pd ₂ Si. |
| | | | | | | | | | | | | | | | | | | | | | Si displaced at interface with silicide. |
| i 111 | | (1×4) | 141 | MEIS | ESA | E | 98 | | < 0.3% | LEED/AES | 3 | 3 | 300 | ? | | ? | 2.352 | | | | Laser annealed (7×7) surface. Results point to |
| | | | | | | | | | | | | | | | | | | | | | surface being disordered patches of (7×7) . |
| i 111 | | (2×1) | 135 | MEIS | _ | н | 99 | _ | _ | | 1 | 1 | _ | | R2v | _ | 2.352 | _ | See No.es | | Tilted pi-bonded chains. |
| i 111 | _ | (2×1) | 136 | MEIS | ESA/MC | н | 99 | | L | LEED/AES | 1 | 1 | _ | 2 | R2v | Several | 2.352 | | See No.es | | Cleaved in vacuum. Tilted pi-bonded chain |
| | | | | | | | | | | | | | | | | | | | | | model [137] best fit. |
| i 111 | | (7×7) | 137 | HEIS | SB | He | 100-4000 | | C/Si < 0.001 | LEED/AES | 2 | Many | 300 | 11 | _ | 300543 | 2.352 | _ | | - | Major reconstruction involves vertical |
| | | | | | | | 1. A | | | | | | | | | | | | | | displacement of 0.4 Å. Lateral strain much |
| | | | | | | | | | | | | | | | | | | | | | smaller than Si(100) (2×1) <0.15 Å. Surface |
| | | | | | | | | | | | | | | | | | | | | | vibrations enhanced by factor of 4. |
| i 111 | | (7×7) | 138 | LEIS | ICISS | He | 0.93 | | | - | Many | Many | - | - | | - | 2.352 | - | - | | Densely-distributed pyramidal clusters of adatoms. |
| i 111 | - | (7×7) | 142 | MEIS | ESA/MC | н | 99 | | | | 1 | 1 | - | 9 | | - | 2.352 | - | See No es | - | Data does not fit pyramidal cluster model, is |
| | | | | | | | | | | | | | | | | | | | | | consistent with stacking fault models |
| | | | | | | | | | | | | | | | | | | | | | [139,140]. |
| i 111 | ~~ | (7×7) | 143 | MEIS | ESA/MC | н | 50-150 | - | LC.O | LEED/AES | 3 | 9 | | 9,11 | | ? | 2.352 | - | - | - | Data consistent with stacking fault models [139-140]. |
| i 111 | Ag | (13×13)R30 | 144 | LEIS | | Ne | 0.5 | 4E + 17 | Trace C | LEED/AES | 1 | 1 | - | _ | | | 2.352 | _ | - | - | Ag atoms slightly embedded below top layer Si. |
| i 111 | Ag | (13×13)R30 | 145 | LEIS | ESA | Ne | 0.5 | ? | L | LEED/AES | - | | 300 | | | - | 2.352 | - | - | - | Room-temperature deposition leads to island growth |
| | | | | | | | | | | | | | | | | | | | | | of commensurate Ag at 0.67 ML coverage. |
| | | | | | | | | | | | | | | | | | | | | | High-temperature (> 200 °C) deposition |
| | | | | | | | | | | | | | | | | | | | | | gives (13×13) structure with Ag embedded |
| | | | | | | | | | | | | | | | | | | | | | in first Si layer. |
| i 111 | Ag | (13×13)R30 | 148 | LEIS | ICISS | Li | 1 | | | - | 5 | Many | - | _ | | - | 2,352 | - | | - | Honeycomb structure above Si layer. |
| (111 | Ag | (1×1) | 147 | MEIS | ESA | H | 175 | | C,O < 0.3% | LEED/AES | 1 | 4 | 300 | | - | | 2.352 | | | - | Deposited on (7×7) surface to give 2 then 3-D |
| | | | | 11510 | | | 1000 | • | 0.200 | | | | 200 | | | | 2.162 | | | | growth. No intermixing, 2 domains. |
| , 111 | Ag | | 146 | HEIS | 5B | He | 1000 | 1 | <0.2%C | MEED/AE5 | 1 | Many | 300 | 12 | | - | 2.352 | | _ | _ | Amorphous nim on (7×7) surface. No mixing |
| | | | 140 | LICIC | | и. | 200 2000 | | | | | Manu | 200 | | | | 2 252 | | | | < 1 ML, for > 5 ML sincide formed. |
| | Ai | - | 149 | AL13 | | L 10 | 000-2000 | _ | _ | | 1 | many | 500 | | _ | | 2.332 | | | | grows enitaxial despite large lattice mismatch |
| ; 117 | A 11 | (13×13)R30 | 150 | LEIS | ICISS | Na | 0.9 | | L | LEED/AFS | 2 | 2 | 300 | _ | _ | | 2.352 | 0.3 | | | Deposition at 700 °C, coverage = 1 ML, An triplet |
| | Au | (13/13/130 | 150 | | | | | - | | | - | - | | | - | | 2.33L | 0.0 | 1 | | clusters on Si honeycomb structure. |
| i 111 | Au | (5×1) | 151 | LEIS | | Nt | 0.5 | 2E + 16 | C/Si = 1/800 | LEED/AES | 1 | 1 | 300 | | _ | | 2,352 | _ · | | | Deposited at 700 °C, coverage 0.4 ML, Au atoms embedded |
| | | | | | | | - | | | | | | | | | | | | | | below outermost Si layer (3 domains). |
| | Au | | 146 | HEIS | SB | He | 1000 | ? | C<0.2% | LEED/AES | 1 | Many | 300 | 12 | | _ | 2.352 | · | _ | _ | Amorphous film on (7×7) surface. No |
| | | | | | | | | | | | | - | | | | | | | | | |

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TABLE 2. Surface structures determined by ion scattering. (continued).

| ubs. Su | rf. | Ads. | Struct. | Ref. | Data Meth. coll. | lon | E(keV) | Dose (m ⁻²) | Cont level | Other tech. | Ang | s. Data | Temp. (K) | Cak | es. R | Debye (K) | d-B (Ä) | d-0 (Å) | d-1 (%) | d-2 (%) | Comments |
|---------|-----|-------|------------|------|---------------------|-----|----------|----------------------------|---------------|----------------|-----|---------|--------------|-----|-------|--------------|------------|-------------|------------|------------|--|
| 11 | 1 | Br | (\3×\3)R30 | 152 | HEIS TC/SB | He | 2500 | L | L | AES | 2 | 2 | _ | - | _ | | 2.35 | 2 0.875(1F) | _ | <u> </u> | 3r adsorbed to thinned crystal from solution |
| | | | | | | | | | | | | | | | | | | | | | 2x situ. Assumed bulk-like substrate. |
| 11 | 1 | Ge | - | 155 | HEIS SB | He | 1000 | ? | L | LEED/AES | I | Many | 300 | 12 | | | 2.35 | 2 — | - | - | Deposited on (7×7) surface at 300-600 °C. |
| | | | | | | | | | | | | | | | | | | | | | At room temperature, amorphous film; |
| | | | | | | | | | | | | | | | | | | | | | at 350 °C, epitaxial growth occurs up to |
| | | | | | | | | | | | | | | | | | | | | | 3 ML; above this strained structure. |
| | | | | | | | | | | | | | | | | | | | | | Above 450 °C intermixing. |
| 111 | 1 | Ni | - | 156 | HEIS SB/TC | He | 1000 | | C<01% | LEED/AES | I | Many | 170,300 | | _ | | 2.35 | 2 — | - | - | - |
| 11 | 1 | NiSi, | (1×1) | 157 | MEIS ESA | н | 100 | | L | LEED/AES | 1 | Many | 300 | 233 | | | 2.35 | 2 | | | Ni deposited on (7×7) surface and heating |
| | | | | | | | | | | | | | | | | | | | | | o 770 K/5 min, to give 25Å-thick |
| | | | | | | | | | | | | | | | | | | | | | NiSi2 film. Ni atoms at interface are |
| | | | | | | | | | | | | | | | | | | | | | 7-fold coordinate and bonds at the |
| | | | | | | | | | | | | | | | | | | | | | nterface are relaxed. |
| 11 | ı | Pd | (\3×\3)R30 | 158 | LEIS — | Ne | 0.5 | | L | LEED/AES | 1 | 1 | 300 | _ | | | 2352 | : <u> </u> | | | 0.5 ML Pd atoms lie below top layer of |
| | | | | | | | | | | | | | | | | | | | | | Si atoms. |
| 11 | 1 | Pd | _ | 146 | HEIS SB | He | 1000 | ? | C<0.2% | MEED/AES | 1 | Many | 300 | 12 | _ | | 2.35 | 2 — | _ | _ | Deposited on (7×7) surface to form |
| | | | | | | | | | | | | | | | | | | | | | ilicides at all coverages. |
| 11 | 1 | Pd | _ | 159 | MEIS ESA | He | 98,174 | | C,O < 0.3% | LEED/AES | 1 | 1 | | | | - | 2.35 | 2. — | <u> </u> | _ | For <1 ML 2-D growth, no mixing. Above |
| | | | | | | | | | | | | | | | | | | | | | 1 ML Pd ₃ Si formation. Attribute |
| | | | | | | | | | | | | | | | | | | | | | differences with [146] to damage. |
| 11 | 1 | Ti | | 160 | MEIS ESA | He | 175 | | C.O < 0.4% | LEED/AES | 1 | Many | 300 | | | | 2.35 | 2 — | _ | _ | I deposited on (7×7) surface. Mixing occurs |
| | | | | | | | | | | | | | | | | | | | | | at room temperature to give TiSi. |
| | | | | | | | | | | | | | | | | | | | | | with may displaced Si atoms at |
| | | | | | | | | | | | | | | | | | | | | | interface. |
| | | | | | | | | | | | | | | | | | | | | | |
| C 00 | ł | 0 | (1×1) | 161 | LEIS — | He | 1 | | O < 1% | LEED/AES | 3 | 3 | 300 | | | | | - | | | O adsorbed on C atoms. |
| 0, 10 | 0 | | c(2×2) | 162 | LEIS CMA | He | 0.5 | ? | L | LEED/AES | 2 | 2 | 873 | | | - | | _ | | _ | Monolayer of O atoms in distorted bridge- |
| | | | | | | | | | | | | | | | | | | | | | bonded zig-zag chains along (100). |
| 0, 110 | 0 | | _ | 163 | LEIS CMA | He | 0.5 | ? | | LEED/AES | 2 | 2 | < 773 | _ | _ | | | | | | Facets above 600 °C. U and O coplanar. |
| 0, 11 | 1 | | | 164 | LEIS CMA | He | 0.5 | ? | L | LEED/AES | 2 | 2 | 873 | | _ | _ | _ | | | | Outermost layer is O occupying bulk-like |
| - | | | | | | | | | | | | | | | | | | | | | positions. |
| 10, 55 | 3 | _ | | 164 | LEIS CMA | He | 0.5 | ? | L | LEED/AES | 2 | 2 | 873 | | _ | _ | _ | _ | _ | _ | Ledge U is covered with excess O. |
| • | | | | | | | | | - | | | - | - | | | | | | | | |
| / 100 | 0 | | (1×1) | 165 | HEIS SB | He | 2000 | - | L C,0 | LEED/AES | 3 | 3 | 300 | 11 | | 384(B) | 1.57 | 8 — | < - 6 | | Signs of disorder at room temperature. |
| 100 | 0 | н | c(2×2) | 166 | HEIS SB | He | 600-2000 | 6E + 18 | - | LEED | 2 | 6 | 300 | 9 | - | _ | 1.57 | 8 — . | - | · | Data not consistent with buckling [234] |
| | | | | | | | | | | | | | | | | | | | | | or zig-zag chains [179b]. |
| 21 | 1 | D: | - | 167 | LEIS CMA | He | 0.3 | ? | L | LEED/AES | 2 | 2 | 300 | — | | - | 1.37 | _ | - | | Beta-2 D_2 thermal desorption state located |
| | | | | | | | | | | | | | | | | | | | | | in deep trough positions. |

.

2F(S) = 2-fold coordinate short-bridge site, e.g., FCC(110)

2F(L) = 2-fold coordinate long-bridge site, e.g., FCC(110).

 $1\Gamma = 1$ fold coordinate site directly on top of another atom

d-1:

The value of the vertical interlayer spacing between the 1st and 2nd layer of the solid expressed in terms of a percentage change from the bulk value. Error in parentheses when given.

d-2:

The value of the vertical interlayer spacing between the 2nd and 3rd layer of the solid expressed in terms of a percentage change from the bulk value. Error in parentheses when given.

The entries used in Table 2 obey the following restrictions:

(1) Articles published in unrefereed conference proceedings or society bulletins were not used.

(2) Papers on thin films and buried interfaces that did not explicitly consider surface structures were not considered.

(3) A series of investigations by the same principal author on the same topic are grouped into one table entry using the latest set of data/results, but all references are provided.

5. Discussion of Structural Results 5.1. Clean Metal Surfaces

Clean metal surfaces were the earliest types of system to be studied by surface crystallographers and interest persists to the present day. Most studies have focussed on the lowindex faces of the face-centered cubic (FCC) metals. The body-centered cubic (BCC) materials W, Fe, and Mo have also received attention, while as yet the hexagonal closepacked metals have not been studied by ion crystallography. For reference, Figure 1 shows the arrangement of surface atoms for some ideal low-index metallic planes.

In the following sections we discuss the surface crystallographic results from ion scattering and LEED. Many metal surfaces closely resemble a truncated bulk lattice, but an increasing number of systems are revealing multilayer oscillatory relaxations. Some surfaces, in particular the (100) and (110) surfaces of Ir, Pt, and Au, exhibit reconstructions that can involve vertical and lateral displacements of atoms from their bulk positions.

5.1.a. Almost Ideal Surfaces

Early LEED studies have shown that, with only a few exceptions, many of the high-density low-Miller-index surfaces of metals do not reconstruct or alter their topmost interlayer spacing (d_1) by more than a few percent (<5%) of the bulk value (d_B) , usually in the form of a contraction. The ion scattering studies of these surfaces have been gathered together in Table 3 with corresponding LEED studies,¹ where available. In general the agreement between ion scattering and LEED results is good, as good as the internal agreement within either technique on its own.

The Pt(111) and W(100) surfaces provide interesting

case histories. Some of the very first channeling studies surfaces were carried out on Pt(111). The initial result of 15% expansion by HEIS¹²⁴ was in strong disagreement wi LEED¹⁷¹⁻¹⁷³ data that showed little or no expansion or co traction. Later HEIS^{121,122} and MEIS¹²⁵ studies agreed wi the LEED results. The initial contradiction was likely due beam damage or contamination.

The W(100) (1×1) surface has received a high degr of attention from LEED workers with a variety of result which eventually have settled down to a value close -7% for d_1 . The HEIS study by Feldman *et al.*¹⁶⁵ on the surface gave a very similar result of a contraction of up 6.7%.

The Pt(100) surface in its clean state is reconstruct (see below); a HEIS study,¹¹⁶ which has not been duplicat using LEED, of a H-stabilized surface showed a nearly ide bulk termination.

5.1.b. Multilayer Relaxed Surfaces

One of the most interesting surface structural results have been discovered recently has been the occurrence multilayer oscillatory relaxations of surfaces such FCC(110), and others with low packing densities. Here take *relaxation* to mean changes in the perpendicular int layer spacings relative to the bulk value, whereas *reconstrutions* involve lateral shifts in atomic position. Several met have been found to exhibit damped oscillatory variations their interlayer spacings, extending sometimes up to 4 lay into the interior of the crystal. Such investigations requir careful approach in order to detect such small structu changes.

A summary of results for such surfaces can be found Table 4. The Ni(110) surface has been extensively studi and has provided some difficulties. This surface was exa ined early in the history of the MEIS technique and founc be bulk-like,⁹⁴ or to have a slightly contracted d_1 (-4%) Later MEIS experiments by Tornqvist *et al.*⁹⁷ confirmed t result, and Feidenhans'l *et al.*,⁹⁶ using HEIS, showed ϵ dence for an expansion of d_2 (+2.4%).

Corresponding LEED studies have also had their d culties. Early work favored contractions of d_1 close to 5 but later investigations produced values of -9% for $d_1 \approx +3\%$ for d_2 .^{184–186}

A further MEIS report from Yalisove *et al.*⁹⁸ found c tractions of d_1 in agreement with the LEED results. ⁵ authors attribute the discrepancy with earlier experiment contamination problems. We can note that the use of blc ing in MEIS studies gives higher sensitivity to multila relaxations than do HEIS rocking curves. Blocking r surements around the appropriate exit direction direyield the change in d_1 ; further measurements in directi which probe deeper into the crystal then give information d_2 . On the other hand, HEIS rocking curves are rather sensitive to multilayer effects, as opposing contraction expansions in the first two layers can reduce the asymmof the rocking curve until it resembles that from an u laxed surface.

The Cu(110) surface provides another example of level of agreement between ion scattering and LEED stuc



FIG. 1. Schematic diagram of the ideal structures of some simple low-index surfaces of metals. In each panel the top and bottom parts are top and side views, respectively. Thin-lined atoms lie behind the plane of thick-lined atoms; dotted lines represent atoms in bulk positions (Ref. 229).

ble 3. Structural parameters^a derived for nearly ideal metal surfaces studied by ion scattering compared with LEED¹.

| ırface | Bulk d _B (Å) | δd ₁ (%) | Method | Ref. |
|---------------------|----------------------------|--|--|--|
| ≥(100) | 1.433 | 0.0 -1.4 | LEIS LEED | 78 231 |
| i(100) | 1.762 | -3.2 0.0 0.0 ± 4.0 0.0 ± 2.5 | MEIS LEED LEED LEED | 82 168 169 170 |
| i(111) | 2.035 | < 1 0.0 0.0 | HEIS LEED LEED | 106 169 170 |
| 1(111) | 2.228 | 0.0 | HEIS LEED | 115 232 |
| 2(100) ^b | 1.981 | 0.0 | HEIS | 116 |
| t(111) | 1.732 | $\begin{array}{c c} -15 \\ < & 2 \\ +1.3 \pm 0.4 \\ +1.5 \pm 1.0 \\ 0.0 \pm 5.0 \\ 0.0 \pm 2.5 \\ +1.0 \pm 0.5 \end{array}$ | HEIS HEIS MEIS LEED LEED LEED | 124 121 122 125 171 172 173 |
| (100) ^c | 1.578 | $\begin{array}{c} <-6.7 \\ -6.0 \pm 1.0 \\ -11.0 \pm 2.0 \\ -5.5 \pm 1.5 \\ -10.0 \pm 2.0 \\ -6.7 \pm 1.0 \\ -8.0 \pm 1.5 \\ -7.0 \pm 1.5 \end{array}$ | HEIS LEED LEED LEED LEED LEED LEED | 165 174 175 176 177 178 179 180 |

xpressed as percentage change from the bulk value

tabilized with H₂

1x1) phase

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HEIS work by Stensgaard *et al.*^{66a} and the studies of Copel *e. al.*⁶⁹ favor a first layer contraction of ~6%, and a second layer expansion of ~2 to 3%. These contrast with the LEIS work of Yarmoff *et al.*,⁶⁷ which produced a value for d_1 of - 10%. LEED studies by Davis *et al*¹⁸³ showed a rather larger value for d_1 of -9% and agreed with d_2 . The HEIS results and further LEED data of Adams and coworkers,¹⁸² showing a similar larger value for d_1 of - 8.5%, were later reconciled.^{66b}

We might also note that in Table 4 there are two ion scattering studies with no LEED counterparts. Strictly speaking, as the Mo(111) investigation⁸⁸ only explored variations in d_1 , we should not include it as an example of multilayer effects. The size of the contraction found (18%) is large enough to make one suspect their presence; however, it should be borne in mind that d_B for Mo(111) is a relatively small 0.90 Å, and hence a large percentage change is not so large in absolute magnitude. Frenken *et al.*¹¹³ also found for Pb(110) an unequivocally large multilayer effect using MEIS; this would be an interesting surface for LEED studies.

5.1.c. High-Index Surfaces

High-index surfaces offer more possibilities for the relaxation of atoms away from their bulk positions. A number of such surfaces have been studied by LEED crystallography,¹ revealing a variety of perpendicular and parallel movements of atoms that still preserve the (1×1) surface symmetry. Studies of such surfaces using ion scattering are just

| Surface | Bulk d _B (Å) | δd ₁ (%) | δd ₂ (%) | δd ₃ (%) | Method | Ref. |
|---------|----------------------------|---------------------|---------------------|---------------------|--------|------|
| Ag(110) | 1.445 | -7.8 ± 2.5 | +4.3 ± 2.5 | | HEIS | 17 |
| •••• | | -9.5 ± 2.0 | +6.0 ± 2.5 | | MEIS | 25 |
| | | -5.7 ± 2.0 | $+2.2 \pm 2.0$ | | LEED | 181 |
| Cu(110) | 1.278 | -5.3 | +3.3 | | HEIS | 66 |
| | | -10 ± 5 | | | LEIS | 67 |
| | | -7.5 ± 1.5 | +2.5 ± 1.5 | | MEIS | 69 |
| | | -8.5 ± 0.6 | +2.3 ± 0.8 | -0.9 ± 0.9 | LEED | 182 |
| | | -9.1 | +2.3 | | LEED | 183 |
| Mo(111) | 0.907 | -18 ± 2 | | | LEIS | 88 |
| Ni(110) | 1.246 | 0 | · | | MEIS | 94 |
| • • | | -4 ± 1 | | | MEIS | 95 |
| | | -4.8 ± 1.7 | $+2.4 \pm 1.2$ | | HEIS | 96 |
| | | -4 ± 1 | | | MEIS | 97 |
| | | -9.0 ± 1.0 | +3.5 ± 1.5 | | MEIS | 98 |
| | | -8.7 ± 0.5 | +3.0 ± 0.9 | -0.5 ± 0.7 | LEED | 184 |
| | | -8.4 ± 0.8 | $+3.1 \pm 1.0$ | | LEED | 185 |
| | | -9.8 ± 1.8 | +3.8 ± 1.8 | | PEED | 186 |
| Pb(110) | 1.750 | -15.9 ± 2.5 | +7.9 ± 2.5 | | MEIS | 113 |

Table 4. Structural parameters^a derived for metal surfaces exhibiting multilayer relaxations by ion scattering compared with LEED¹.

 a expressed as percentage change from the bulk value d_B

starting to appear in the literature e.g. Cu(410),⁷⁴ Cu(16,1,1),⁷⁶ Pt(997).¹²⁶

5.1.d. Reconstructed Surfaces

The (110) surfaces of Au, Ir, and Pt exhibit a (1×2) reconstruction when clean. The Au surface in particular has been the subject of numerous ion scattering and LEED investigations. A number of possible surface structures have been proposed involving hexagonal close-packed overlayers, paired rows, buckled, and missing rows. In general the consensus appears to favor a structure with a missing row of atoms in the [-110] direction in the surface leading to a doubling of the unit cell in the [001] direction as shown in Fig. 2. The Au surface structure seems to be the best established with a large contraction of the 1st layer, a small lateral pairing displacement of the 2nd layer and a possible buckling of the 3rd layer. The existence of the missing row does not seem to be in doubt, it having been also seen by electron microscopy,¹⁹⁰ and the scanning tunneling microscope.¹⁹¹ However, some differences in detail exist between MEIS,^{56,60} HEIS,¹⁶ and LEED¹⁸⁷ results (See Table 5).



FIG. 2. Schematic diagram of the missing-row model of the (2×1) reconstructed (110) surfaces of Au, Ir, Pd and Pt.¹⁸⁷

LEED studies of $Ir(110)^{188}$ found the missing remodel with a large contraction of the 1st layer spacing, sir lar to that in Au(110), to produce a slightly better fit that row-pairing or buckled-surface model. The correspondi MEIS study,⁶⁰ on an apparently only partially reconstruct surface, was in agreement with the overall structure.

The position for Pt(110) is less clear. A LEED study and LEIS ¹¹⁹ work again tended to favor a missing-row rangement, while an HEIS investigation by Jackman *et al.* concluded that their data excluded any significant late displacements or vertical shifts. Rocking scans both norn and off-normal to the surface were extremely symmetri implying that any lateral movement from bulk positions h to be <0.02 Å, and vertical shifts of <0.07 Å. This d suggests that the Pt(110) and Au(110) reconstructions a possibly rather different; the HEIS data is consistent with unrelaxed, or very weakly buckled, surface.

The normal (1×1) W(100) surface undergoes a tr. sition to a reconstructed $c(2 \times 2)$ form below 300 K, or exposure to hydrogen. Two HEIS studies^{165,166} agree w LEED data^{192,193} in finding a small contraction in d_1 . 1 LEED structure of Debe and King¹⁷⁹ has atoms in the [11 direction forming a zig-zag row structure as shown in Fig The ion scattering results of Stensgaard *et al.*¹⁶⁶ indicate t about one-half of a monolayer of atoms have shifted po tion. This is consistent with the zig-zag chain model if recstructed domains coexist with bulk-like areas that are sta lized by some surface defect.

5.2. Adsorbate-Covered Metal Surfaces

The variety of adsorbate systems that have been stud by ion scattering is rather small. Most investigations h involved O or S chemisorption, most usually on Cu and

Table 5. Structural parameters from ion scattering and LEED for the missing-row structure for the (1x2) reconstructed (110) surfaces of Au, Ir and PL^a.

| | d _B (Å) | d ₁ (Å) | d2 (Å) | d3 (Å) | δz3 (Å) | δy1 (Å) | Method | Ref. | |
|----------------------|-----------------------|-----------------------|-----------|-----------|------------|------------|--------|-------|--|
| | | | | | | | | | |
| Au(110) | 1.442 | 1.19 | | | | <0.1 | LEIS | 59 | |
| | | 1.18 | 1.49 | | 0.10 | <0.1 | MEIS | 56,60 | |
| | | 1.19 | | | | 0.18 | HEIS | 16 | |
| | | 1.15 | 1.35 | 1.35 | 0.23 | 0.07 | LEED | 187 | |
| Ir(110) | 1.352 | 1.23 ^b | , <u></u> | | | | MEIS | 60 | |
| | | 1.16 | 1.16 | | <0.2 | <0.2 | LEED | 188a | |
| | | 1.19 [°] | 1.20 | 1.28 | 0.23 | 0.10 | LEED | 188b | |
| Pt(110) ^d | 1.387 | 1.39 | | | <0.02 | <0.07 | HEIS | 120 | |
| | | 1.7 | 1.38 | | | 0.05 | LEED | 189 | |
| | | | | | | | | | |

^a parameters are defined in Figure 2.

^b surface apparently not homogeneous

^c paired rows in second layer, and buckled rows in third layer

^d data consistent with very weakly buckled surface

cause of their small cross sections for scattering, adsortes such as C and O are difficult to detect by shadowing d blocking. However, the changes in blocking patterns are ten sufficient to establish the location of the adsorption e, and the height of the adatom above the surface d_0 .

There appears to have been only one true case of molecar adsorption studied, that of CO/Ni(111).¹⁰⁷ This experient showed the CO bonded through the C atom as has been ind in many other metal/CO systems by LEED.¹



W (100) - c (2 x 2)

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5.2.a. Simple Atomic Adsorption

In the main, atomic species adsorbed on low-index surfaces have been found to occupy the high-symmetry sites shown in Fig. 4. Sometimes adsorption is accompanied by rearrangements of the substrate as discussed below, but often the chemisorption appears to be simple. This simplicity may be more apparent than real as many LEED and ion scattering studies have assumed that chemisorption did not induce reconstruction.

The adsorption sites are described in Table 2 as XF, meaning X-fold coordinate, considering only the 1st shell of nearest neighbors. In some cases, alternate sites of the same coordination are distinguished by the arrangement of metal atoms making up the site, e.g., 2F(S) and 2F(L)-short and long 2-F bridge sites on an FCC(110) surface.

Table 6 summarizes the ion scattering and LEED results for these systems. There is almost perfect agreement between the two techniques on adsorption sites, and d_0 values agree within a small margin. The Cu(100)-O system has presented difficulties and probably involves penetration of O atoms into the surface, particularly at higher coverages.

5.2.b. Adsorption-Induced Surface Reconstruction

Changes in the geometry of substrate atoms due to adsorption fall into two classes: alteration, usually removal, of a reconstruction or relaxation pre-existing on the clean surface, or the formation of a new reconstruction of the metal atoms.

The removal of a clean surface reconstruction upon adsorption has been followed in a few cases by ion scattering. The best examples involve platinum. The conversion of the (1×2) Pt(110) and the Pt(100) (5×20), or "hex", recon-

FIG. 3. Schematic diagram of the W(100) $c(2\times 2)$ reconstructed surface structure (Ref. 230).





(a) fcc(111), hcp(0001): hollow site





(b) bcc(110): 3-fold site



++++

(c) fcc(100) hollow site





(d) bcc(100): hollow site









(f) hcp (0001): underlayer

FIG. 4. Schematic diagram (top and side views) of high-symmetry adsorption sites on low-index surfaces of metals (Ref. 229).

| Surface | Adsor- bate | Struct- ture | Site | d _o (Å) | Method (Å) | Ref. |
|----------|----------------|-----------------|--------------|--------------------|-------------------|-------|
| 2~(110) | | (27) | 2 1 1 | | TRIC | 40 |
| AG(110) | 0 | (2X1) | 26-0 | | LEED | 194 |
| Cu(100) | ο | C(2x2) | 2F/4F | | LEIS | 32,64 |
| | | | 2F? | 1.4 | LEED | 195 |
| Fe(100) | 0 | (1x1) | 4F | 0.56 | LEIS | 79 |
| | | | 4F | 0.48 | LEED ^a | 196 |
| Ni (100) | D | | 4 F | 0.5 | HEIS | 90a,b |
| | ο | c(2x2) | 4F | 0.90 | LEIS | 92 |
| | | | | 0.86 | MEIS | 89 |
| | | | | 0.90 | LEED | 197, |
| | | | | 0.80 | LEED | 199 |
| | S | c(2x2) | | 1.40 | LEIS | 93 |
| | | | | 1.30 | LEED | 200- |
| | | | | | | 202 |
| Ni(110) | S | c(2x2) | 4F | 0.87 | MEIS | 105 |
| | | | | 0.89 | LEIS | 93 |
| | | | | 0.84 | LEED | 203 |
| Ni(111) | со | (2x2) | ^c | | LEIS | 107 |

Table 6. Adsorption sites and distances for systems showing no reconstruction due to adsorption determined by ion scattering and LEED.

^a also found $d_1 = -7.5$ %

^b probable reconstruction

^c adsorbed through C atom

structions to (1×1) by hydrogen or CO were studied by the Chalk River group.^{116,120}

Many metals show significant changes in the degree of relaxation of their surface layers on adsorption by ion scattering and LEED. They are summarized in Table 7.

The most interesting feature of Table 7 is that expansion of the surface upon adsorption of 0.5 monolayers of O or S appears to be common. On clean surfaces that are contracted, the expansion induced by adsorption can be great enough to result in an overall expansion of d_1 . Thus the MEIS experiments of van der Veen *et al.*¹⁰⁵ showed that the 8% contraction of clean Ni(110) turned into a 5% expansion with 0.5 monolayers of adsorbed sulfur.

Adsorbate-induced reconstructions of the underlying substrate atoms are becoming a feature of surface crystallography. Two prominent cases that have been extensively investigated by the ion scattering community are the (2×1) O-induced reconstructions of Cu and Ni(110).

The Ni(110) (2×1) reconstruction has generated a significant amount of discussion. Early LEIS work by Verheij *et al.*¹⁰⁰ indicated the presence of a reconstruction and identified the adsorption site as a long-bridge site. Later MEIS shadowing/blocking studies by Smeenk *et al.*¹⁰¹ gave strong evidence for a missing-row reconstruction. This has been further supported by ICISS work by Niehus and Comsa,¹⁰³ while Schuster and Varelas¹⁰² have suggested a saw-tooth modification.

For Cu(110), LEIS results^{67,70} suggest a missing-row structure, while HEIS studies⁷¹ prefer a buckled-row model. It may well be that the differences between investigations will boil down to the fact that the exact condition of the surface in the case of these adsorbate-induced reconstructions depends critically upon the method of preparation. There is evidence that the temperature of exposure may be a crucial variable.²

5.3. Semiconductor Surfaces 5.3.a. Silicon Surfaces

The cleaved Si(100) surface exhibits a (2×1) LEED pattern indicative of a reconstruction. Adsorption of hydrogen results in a (1×1) pattern that has been shown to be due

to an essentially truncated bulk structure by both MEIS^{127,129} and LEED.²⁰⁴

The (2×1) reconstruction has been the subject of i number of studies. Models for the surface geometry have basically revolved around two concepts—either surface vacancies, or dimerization of surface atoms, similar to the paired-row and missing-row models for Au(110). A number of these models are shown in Figure 5.

An ICISS study by Aono⁴¹ found evidence for surface dimers; in addition LEED²⁰⁵ and STM²⁰⁶ evidence also pointed to surface dimerization as being the correct model. A MEIS study by Tromp *et al.*¹²⁸ found that models involving symmetric dimers did not fit their data. Blocking patterns taken in various scattering geometries were in agreement with a buckled or asymmetric dimers,¹³¹ in which one of the paired atoms sinks deeper into the surface than the other, and also included subsurface distortions. This model has the added attraction that the occasional finding of $c(4\times 2)$ LEED patterns can be explained by suitable arrangements of these buckled dimers.

The most recent LEED^{207,208} experiments and the transmission HEIS work of Jin *et al.*¹³⁰ confirm this general picture, but find that a twisting of the asymmetrical dimer around an axis perpendicular to the surface improves the agreement with experiment. This model is shown in Fig. 6, and crystallographic data collected in Table 8. Unfortunately, total energy calculations^{128,209} for the Yang *et al.* model²⁰⁸ indicate that displacements perpendicular to the (110) plane are destabilizing. Hence, although the major features of the Si(100) (2×1) surface appear to be under control, the fine details are in doubt.

The (111) surface of Si has been one of the most studied of all surfaces in surface science, and it has received due attention from the practitioners of ion scattering. The vacuum cleaved surface shows a (2×1) LEED pattern that evolves to a (7×7) structure after annealing. The surface relaxes to a (1×1) structure if laser annealed, or quenched at high temperatures. It can also be stabilized by small amounts of impurities such as Te.

Many models involving buckling, 210,211 molecular 212 and pi-bonded chains, 213 and conjugated chains 214 have been proposed to account for the (2×1) LEED pattern observed

Table 7. Relaxations of metal first interlayer spacings upon adsorption⁴, determined by ion scattering and LEED.

| Metal | δd₁ (%) clean surface | Adsorbate | δd ₁ (%) after ad- sorption | Method | Ref. |
|---------|-----------------------------|-----------|--|--------------|------------|
| Ni(100) | 0 | c(2X2)-0 | +5.2 | MEIS | 89 |
| Ni(110) | -8.4 | c(2X2)-S | +6 +10 | MEIS LEED | 105 203 |
| Ni(111) | 0 | (2x2)-0 | +7.4 | HEIS | 106 108 |
| Pt(111) | 0 | (1x1)-CO | +0.8 | HEIS | 120 |

^a Expressed as percentage changes from the bulk value d_B.

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Table 8. Atomic geometry of buckled dimer models of the Si(100) (2X1) surface^a.

| | Yin ar | Yin and Cohen ¹⁰⁴ | | | Yang et al ²⁰⁸ | | | |
|--------------------------------------|-----------------|------------------------------|-----------------|-----------------|---------------------------|---------------|--|--|
| Atom | δx | δy | δz | δx | δy | δz | | |
| Si ₁₁ Si ₁₂ | -0.520 1.040 | 0 0 | 0.160 | -0.650 0.750 | -0.300 0.300 | 0.04 0.44 | | |
| Si ₂₁ Si ₂₂ | -0.094 0.115 | 0 | 0.047 -0.020 | -0.060 0.120 | -0.100 0.100 | 0.13 0.13 | | |
| Si ₃₁ Si ₃₂ | 0 | 0 0 | -0.139 0.185 | 0 0 | 0 | -0.15 0.20 | | |

^aParameters are defined in Figure 6.

tilted π -bonded chain

FIG. 5. Different models proposed for the Si(100) (2×2) reconstruction. (Ref. 2).



FIG. 6. Schematic diagram of the asymmetric dimer geometry of the (2×1) structure of Si(100) (Ref. 207). (a) Projection of the 2×1 unit cell on {110} plane of bulk Si $(a_x = 7.68 \text{ Å}, a_y = 5.44 \text{ Å})$. (b) Projection of the 2×1 unit cell on the {001} plane of bulk Si $(a_y = 3.84 \text{ Å})$. from cleaved Si(111). Two MEIS studies^{135,136} agree w the most recent LEED study²¹⁴ in favoring a modified bonded chain model in which the outer chain is buckled w an overall compression. This structure is detailed in Fig and Table 9.

The (7×7) reconstruction of Si(111) has been a matchallenge to surface scientists. Ion scattering studies¹³⁷ have played a significant role in unravelling this structure fact this surface has shown the value of combining the immation available from many different surface science te niques.

Because of the size of the (7×7) unit cell, early k matic LEED studies on this surface produced a large nu ber of competing models for the structure (see Ref. 216 Refs. therein). The first HEIS experiments by Culbertso *al.*¹³⁷ required unreasonably large perpendicular displiments of up to 0.5 Å for the atoms in the first two layers. 7 data was reanalyzed by Bennett *et al.*¹⁴⁰ in terms of a staing fault dividing the surface up into triangular areas. 7 idea was enlarged upon by Himpsel and Batra²¹⁵ McRae,¹³⁹ who noted that the topological requirement joining double layers at the subunit boundaries should 1 to arrays of dimers and deep holes. Further MEIS exp ments by Tromp and van Loenen^{142,143} support the stack fault model and showed that the LEIS results of Aon*al.*¹³⁸ could be interpreted in these terms.

The situation was clarified by the transmission elect diffraction experiments of Takayanagiet *al.*,²¹⁷ and the r space images provided by Binnig *et al.*²¹⁸ using the scanr tunneling microscope. These results, coupled with the lier ion scattering and LEED data were reconciled in dimer-adatom-stacking fault (DAS) model shown in Fi In this model, the outermost double layer consists of triangular subunits which are, respectively, faulted and faulted with respect to the substrate. The partial dislocat at the border of the triangular subunits are reconstruinto 12-membered rings surrounding a corner hole 6.



FIG. 7. (a) The buckled and pi-bonded chain models for the Si(111) (2×1) reconstruction (Ref. 230). (b) Schematic diagram of the buckled pibonded chain model for the (2×1) structure of Si(111) showing a side view (Ref. 214).

deep, together with alternating dimers and 8-membered rings.

The DAS model has come to be generally accepted as containing all the correct ingredients of the (7×7) structure, but some important information remained missing, e.g., vertical distances between atoms. Employing a new theoretical approach, Tong *et al.*²²⁰ have performed a full

LEED analysis on this structure and produced a refined version of the DAS model. This model, which contains the coordinates for 200 atoms in the first five atomic layers, shows an oscillatory relaxation with atomic planes having stretched bonds followed by ones in which the bonds are compressed.

The Si(111) (7×7) reconstruction can be quenched to (1×1) by the presence of impurities, or laser annealing. Tromp *et al.*¹⁴¹ found by MEIS that the laser annealed (1×1) surface shared many of the basic structural features of the (7×7) reconstruction, possibly consisting of disordered areas of the reconstructed material. This result contradicted an earlier LEED study of Zehner *et al.*²²¹ that favored a bulk-like surface with a contracted first layer spacing. A later LEED study, however, found as good agreement with a graphitic top double layer of Si atoms.²²²

5.3.b. Si/adsorbate Systems

Studies of adsorbed gas phase species on Si by ion scattering are relatively rare. H and D adsorption on Si(100)^{127,129} and (111)¹⁵⁴ have been valuable in understanding the reconstructions of these surfaces. There is also an interesting transmission HEIS study by Gibson and coworkers¹⁵² of bromine adsorbed from a bromine/ethanol solution onto Si(111), which found the halogen to be bound directly over the first layer Si atoms.

Much of the recent work in channelling has been directed towards understanding the growth of metallic thin films on Si surfaces, particularly those used in electronic device manufacture. Important goals are to characterize the growth mode, defect formation, and the nature of buried interfaces. Such studies are in general not included here, but there are a number of investigations in this area that have defined the early stages of growth and provided surface structural results.

The largest number of ion scattering studies concern the growth of the noble metals Ag and Au on Si(111) and (100); there are few LEED counterparts. Both HEIS, ^{134,136} MEIS,¹⁴⁷ and LEIS^{144,145,148,150,151} have shown little intermixing of the elements at room temperature for coverages up to a monolayer. Silicide formation occurs at higher coverages. 134,146 Heating a Si(111) (7 \times 7) surface that contains a monolayer or so of Ag results in a $(\sqrt{3} \times \sqrt{3})$ R30° structure that has been studied by two different groups using LEIS, with differing conclusions. Saitoh et al. concluded, from ICISS^{144,143} and LEED,²²³ that Ag atoms were slightly embedded below the topmost Si layer [Figure 9(a)]. Aono and coworkers¹⁴⁶ interpreted their ICISS data as a honeycomb arrangement of Ag atoms located above the first Si layer [Figure 9(b)]; Oura et al.¹⁵⁰ have proposed a similar structure for the analogous Au $(\sqrt{3} \times \sqrt{3})$ R30° system.

The interaction of Pd with Si surfaces appears to be qualitatively different in that spontaneous formation of a mixed Pd–Si layer occurs with the composition Pd_2Si .^{49,159} For Ti, MEIS measurements show that the mixing occurs at room temperature to give TiSi, which then becomes coated with a pure Ti layer upon further adsorption.¹⁶⁰

Table 9. Atomic geometry for the buckled pi-bonded chain model of Si(111) (2x1) structure^a.

| Atom | Х | Y | z |
|----------------|------|------|-------|
| 1 [.] | 1.09 | 1.92 | -3.90 |
| 2 | 4.45 | 0.0 | -3.93 |
| 3 | 2.21 | 0.0 | -3.23 |
| 4 | 5.54 | 1.92 | -3.08 |
| 5 | 2.22 | 0.0 | -0.89 |
| 6 | 5.54 | 1.92 | -0.69 |
| 7 | 0.09 | 0.0 | -0.02 |
| 8 | 3.24 | 1.92 | -0.09 |
| 9 | 0.95 | 0.0 | 2.18 |
| 10 | 2.34 | 1.92 | 2.11 |
| 11 | 4.34 | 1.92 | 3.37 |
| 12 | 5.46 | 0.0 | 2.99 |

^aThe x,y,z coordinates (Å) refer to the [-12-1], [-101], and [111] directions shown in Figure 7 with the origin at a third layer atom of the truncated bulk lattice²¹⁴.

5.3.c. III-V Semiconductors

The cleavage (110) surface of III-V semiconductors is nonpolar and retains the (1×1) surface unit mesh expected for a truncated bulk structure. However, it was soon discovered that GaAs(110) is in fact reconstructed in a subtle



FIG. 8. Schematic diagram of the Si(111) (7×7) structure. (a) first three layers in plan view showing joining of double layers at the edge of a triangular island. Dimers are formed by pairing atoms common to each pain of 5-membered rings (Ref. 219). (b) Plan view showing the stacking fault (shaded area), prominent depressions in the surface (round and oval holes), and dimers (double lines) (Ref. 139a). manner. The solution of this structure became something a cause célèbre in the LEED community.

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Initial LEED work suggested two models where t surface is relaxed from its bulk configuration through bo rotations (ω in Fig. 10 in the first bilayer.) In the bor rotation model²²⁴ a rotation of ~27° allowed for conserv tion of bond lengths. The alternative bond-relaxation more needs a much smaller rotation angle of 7°.²²⁵ Further LEE work favored the bond-rotation structure.²²⁶







FIG. 9. (a) Model for Ag atoms embedded below topmost Si(111) layer $(\sqrt{3} \times \sqrt{3})$ R30° structure (Rcf. 145). (b) Model for Ag atoms adsorbed honeycomb arrangement above topmost Si(111) layer $(\sqrt{3} \times \sqrt{3})$ R30° structure (Ref. 146).





FIG. 10. (a) Schematic diagram of the relaxed zincblende (110) surface (Ref. 231). (b) View of the GaAs(110) (1×1) reconstructed surface. From (Ref. 230).

Although an early HEIS study⁸² agreed with the bond relaxation 7° model, later MEIS measurements by Smit *e al.*⁸³ reaffirmed a bond length-conserving rotation of 29° These authors attribute the conflict with the HEIS work t₀ more careful surface preparation.

The bond length conserving structure for III-V (110) surfaces has been further strengthened by the finding of similar approximately 30° rotations for GaSb and InAs (see Table 10).

The GaAs(100) surface shows a large number of complex reconstructions that are dependent upon the Ga/As ratio in the surface after preparative procedures. A HEIS study⁸¹ has indicated that the H-saturated surface relaxes to a bulk-like geometry. The same study found for the $c(4\times4)$ surface significant lateral displacements of surface Ga and As, atoms and subsurface strain.

5.4. Other Nonmetal Surfaces

The number of ion scattering studies on surfaces on nonmetals other than semiconductors are rather small, and often not very complete. They include: diamond,⁶¹ LaB₆,^{86,87} and UO₂.¹⁶²⁻¹⁶⁴

The most complete of these investigations is that of Derry *et al.* on diamond,⁶¹ both H-terminated (1×1) and reconstructed (2×1) . MEIS showed the H-terminated surface to be bulk-like and unrelaxed (within 0.05 Å), in good agreement with LEED data.⁶³ The scattering from the (2×1) reconstructed surface was consistent with a pi-bonded chain structure of the type seen on the equivalent Si surface.

| | Layer | δ_{ai} | δc_1 | $\delta \mathbf{a}_{\parallel}$ | $\delta \mathbf{c}_{\parallel}$ | ω | Method | Ref. |
|--------|-------|------------------------|----------------|---------------------------------|---------------------------------|-------|--------|---|
| | | (Å) | (Å) | (Å) | (Å) | (deg) | | |
| | | | | | | | | ~ |
| GaAs | 1 | 10.12 | 10.06 | ≤0.1 | ≤0.1 | 7 | HEIS | 82 |
| | 2 | 10.03 | 10.03 | 0.0 | 0.0 | | LEED | 225 |
| | 1 | t0.14 | ↓0.51 | -0.33 | -0.49 | 27 | LEED | 222 |
| | 2 | 10.06 | 10.06 | 0.0 | 0.0 | | | 226 |
| | 1 | 10.20 | ↓0.51 | -0.34 | -0.51 | 29 | MEIS | 83 |
| C . Ch | 2 | | 10 55 | | | | | |
| Gasp | 2 | 0.0 | +0.55 | ~0.38 | -0.58 | 30 | LEED | 227 |
| | - | | | | | | 5650 | |
| InAs | 1 | 10.22 | ↓0.55 | -0.36 | -0.57 | 30 | MEIS | 85 |
| | | | 10 50 | 0.10 | 0 67 | | 1000 | 220 |
| | 2 | 10.22 | +0.56 t0.07 | -0.13 | -0.57 | 31 | LEED | 228 |

Table 10. Atomic geometries of zincblende (110) surfaces determined by ion scattering and LEED crystallography^a.

^aParameters are defined in Figure 10.

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