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SURFACES AND DISORDER

Proceedings of the 12th Midwest Solid State Theory Symposium, held in St. Paul, Minnesota in September, 1984.

Guest Editor: J. W. Halley

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PREFACE

The 12th annual Midwest Solid State Theory Symposium held in St. Paul, Minnesota in 1984 attracted a very high quality of both young and established theorists from academic and industrial institutions. Though the symposium had not been planned with a theme, the contributions of the speakers complemented each other very nicely. For the proceedings, we have asked the speakers to make their contributions as pedagogically readable as possible and we think that they have largely succeeded. The result reviews a wide but related set of current interests in condensed matter theory.

We first present papers based on the talks by L. W. Burch, John Smith and Jack Dow on surface phases, adhesion and Schottky barriers in which the underlying model of the surface is planar. In the next contributions, on the Laplacian roughening model, equilibrium crystal shapes and dendritic growth by David Bruce, Michael Wortis and Eschel Ben-Jacob respectively one studies decidedly non planar interfaces. This leads naturally to descriptions of material in the talks by Joseph Straley, Rajiv Kalia, and P. L. Taylor on structure of defects in glasses, two dimensional glasses and polymers. Finally, we have papers on the classical dynamics (in networks by Michael Thorpe and in diffusion on fractals by Hisao Nakanishi) and the electron dynamics (based on talks by C. M. Soukoulis, Barry Kunz, Mike Lee, David Stroud, and Craig Davis) of disordered systems.

The symposium is an informal conference designed for the pleasure and enlightenment of the participants and particularly for the students and young investigators among them. It is our hope that these proceedings will serve similar purposes for their readers.

We are grateful to the Argonne Universities Association, the Graduate School and Physics Department of the University of Minnesota and Argonne National Laboratories for supporting the symposium financially. The symposium also owed much to Zlatko Tesanovic and David Price, who served on the local committee, to the participants including especially the more than 25 who contributed to the poster session and to Lockwood Carlson of 3M company, who discussed the role of theoretical physics in industry in a well received afterdinner talk.

J. WOODS HALLEY
March 12, 1985

Minneapolis, Minnesota

TABLE OF CONTENTS

Materials Science Forum, Volume 4 (1985), pp. 1-20.

STRUCTURE OF THIN PHYSISORBED LAYERS

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ABSTRACT

This paper is based on a talk presented at the 12th Midwest Solid State Theory Symposium. It gives an overview of results on the structure of thin layers of inert gases and small linear molecules presented in several recent papers by the author and his co-workers. Uniaxial registry monolayers and the theory of the monolayer to bilayer solid transition are treated. Some qualitative remarks to place the work in the context of other work on multilayer growth and on registry effects in monolayers are included. The work of other authors is not systematically reviewed but references to several of the major papers are included.

1. INTRODUCTION

Thin physisorbed layers of inert gases and small linear molecules--one, two, and three-layer films--show a wide range of phenomena and may be well-suited for a systematic study of modes of crystal growth [1]. There are many examples where the adsorbate- adsorbate interactions in the form known from study of the bulk phases contribute the major part of the lateral cohesive energy of the adsorbed film [2]. There are also examples [Xe and Kr on Pd(100)] where the dispersion force attractions seem to be thoroughly disrupted or compensated in the first layer [3]. The competing periodicities of the "intrinsic" adsorbed lattice, which would be formed on an atomically smooth substrate, and of the actual substrate surface lead to a variety of registry and near-registry structures [1,4].

We will follow the evolution of several adsorbate/substrate combinations from condensation of the first layer to the formation of the 2-layer and 3-layer films. The simplest pattern is observed for Xe on the (111) face of the face-centered cubic metal silver, Xe/Ag(111) [5,6]. The monolayer lattice

constant varies by a small but measurable amount before the bilayer is formed and the lateral stresses arising from the compression make a large contribution to the monolayer chemical potential [7]. Indeed, when the compressibility is explicitly included in the analysis, we arrive at a qualitative understanding of the similarity of the bilayer condensation chemical potential for a given adsorbate on several substrates [3,5,8]. Although one might have viewed the first layer holding potential as setting the "origin" or "zero" of the chemical potential, the chemical potential at the bilayer formation is only weakly dependent on the first layer holding potential.

There is much interest in the approach to bulk properties as thicker films are formed [9-17]. For the system Xe/Ag(111) [5] the lateral nearest neighbor spacing L of the Xe atoms at monolayer condensation was 2% larger than the spacing L_s in bulk Xe at its sublimation curve at the same temperature.At and beyond the second layer formation the spacing L was indistinguishable from L_s, i.e., they were equal to 0.2%. This led to a belief [5,7] that for Xe/Ag(111) one could grow arbitarily thick films continuously, that Xe/Ag(111) followed the Frank-van der Merwe mode of crystal growth [14]. In some other adsorption systems involving inert gases and small molecules the continuous growth is apparently not achieved [15,16]. The layer-plus-island, or Stranski-Krastanov, growth mode [14] is proposed to occur for several linear molecules on the basal plane surface of graphite (Gr) and for adsorbed layers with large quantum effects (Ne/Gr and He/Gr) [15]. A qualitative discussion can be given [14] of effects which enhance the likelihood for the Stranski-Krastanov mode to occur: "almost any factor which disturbs the monotonic decrease in binding energy, characteristic of layer growth, may be the cause." Structural considerations provide a guide: registry, symmetry, and compression each play a role. The model calculations of monolayer structures will be discussed here in this context.

A related subject, which we do not treat here, is the development of electronic structure in thin metal overlayers [17].

The presentation is organized in four parts. In Section 2 the phenomena for two-dimensional solids, i.e., monolayer solids adsorbed on smooth planar surfaces,are summarized. Experimental systems which exhibit such intrinsic monolayers include Xe/Ag(111) [5] and Ar/Gr [18]. In Section 3 the monolayer packing problems for molecules with shapes, such as linear molecules [19,20,21,22], are discussed. In Section 4 registry and near-registry monolayers on adsorbing surfaces with rectangular symmetries are discussed. This includes systems such as Xe/Ag(110) [23], Kr/Cu(110) [24,25], and Xe/Cu(110) [23,25] for which the observations of registry structures have been used [26] to estimate the lateral corrugation of the holding potential. Finally in Section 5 recent work and speculations [27] for compressed monolayers are discussed, including the special features arising for adsorbed helium as a consquence of the large variations in the holding potential between substrates [28,29,30].

2. Two-Dimensional inert Gas Solids

In this section we discuss the observations on and modelling of the intrinsic, close-packed monolayer solids of physisorbed inert gases. As is the case for the three-dimensional solids [31], the inert gases condense in rather simple structures in which most of the cohesive energy is the result of pairwise interactions. Knowledge of the pair potential from the dilute

three-dimensional gas phase transfers to the 3D solid and, in large part, to the adsorbed layers [2]. Also in analogy to the case of the three-dimensional solids, there is a strong interplay in the analysis between the development of the statistical mechanical theory for calculating thermal properties and the determination of the full interatomic potential as modified by substrate-mediated processes in the adsorption. The experimental systems which are studied by diffraction on single crystal substrates and which most closely follow the model of a monolayer solid on a smooth dielectric continuum adsorbing surface are Xenon, Krypton, and Argon adsorbed on Ag(111) [5,6,32] and Argon and Neon adsorbed on Gr [18,33,34].

A characteristic of the physisorbed monolayers is that a continuous variation of the adlayer lattice is experimentally possible [5]. The layer can be manipulated by adjusting the temperature and pressure of coexisting 3D gas and its response (e.g., compressibility) can be measured. At monolayer condensation, which occurs at the 2D sublimation curve, the diffraction experiments provide values for $L_o(T)$, the lattice constant of the essentially unconstrained (zero spreading pressure) monolayer solid, and also measures of the density of the coexisting 2D gas at temperatures not far from the supposed 2D triple point. A thermodynamic path followed in such experiments is shown in Figure 1, which is the phase diagram of Xe/Ag(111) [5]. The path ABC, at constant pressure and decreasing temperature, goes from condensation from a dilute 2D gas to a 2D solid (at line a) through a region of monolayer solid (along AB) to the condensation of bilayer solid (at line b) and then on to the appearance of 3D solid (at line c, the bulk sublimation curve). Support for this interpretation of the state of the adsorbed layer is shown in Figure 2, taken from the work of Unguris [5]: Figure 2a shows the adsorbate coverage/area derived from the attenuation of a diffraction signal from the underlying substrate, while Figure 2b shows the combination of these data with the measured lateral nearest-neighbor spacings L in the form of an adsorbed area (coverage times L^2). The slight slope to the long plateau in Figure 2a (region AB of Figure 1) is absent in Figure 2b and the adsorbed area at B, bilayer formation, is twice that along the plateau, to 1%. This analysis led to the identification [5,7] of the Xe/Ag(111) few-layer solids as particularly clean experimental systems with very few vacancies. The slight rise before the monolayer condensation in Figure 2a corresponds to a 2D gas of density 10% of the monolayer solid, an intriguing gas which has been discussed at length elsewhere [35].

The bilayer formation can be viewed as the condensation, under increase of chemical potential, of the dilute thermally activated second layer gas which is present even for the monolayer solid. In computer simulations [36] of the Xe/Gr system at temperatures above 100 K, such gas of density more than 10% of the first layer solid is seen. Modelling of the lower temperature solids represented by Figure 2 has the simplifying feature that the second layer gas density prior to bilayer formation is quite dilute. The statistical mechanical theory of the monolayer to bilayer transition at intermediate temperatures includes effects of vacancies in the solid layers and of the second layer gas of the monolayer solid [37].

A consequence of the compressibility of the monolayer solid is that there is not a unique monolayer lattice constant: for Xe/Ag(111) the lattice constant at monolayer condensation is 1.8% larger than the near-neighbor spacing L_s in the 3D solid at the bulk sublimation curve, while at the bilayer formation the lattice constant is within 0.2% of L_s [5]. With the precision being achieved in measurements of the lattice constant [5,6], it is important to compare

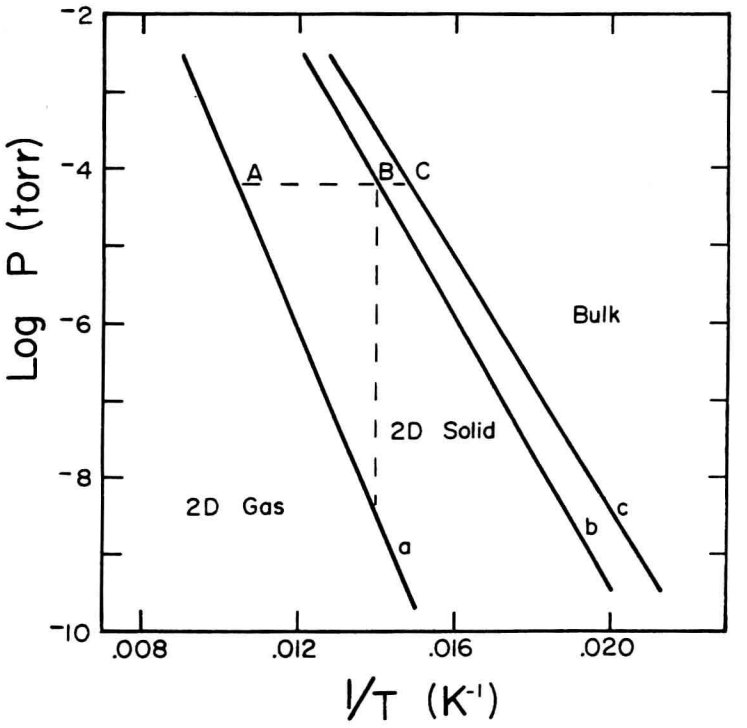


Figure 1. A portion of the phase diagram for Xe/Ag(111). The coordinates are the pressure p of a coexisting 3D gas and temperature T. The dashed lines denote paths of isobaric compression (ABC) and isothermal compression.

results at the same state of the phase diagram. In particular, small differences in the coverage (a few percent) can make large difference in the compression.

The statistical mechanical theory of the monolayer solid has been developed in various approximations [38-42]. The adatom-adatom interactions include the pair potential known from the analysis of 3D phases and several substrate mediated interactions. The parameters for the interactions of adsorption induced dipoles and for the substrate modifications of the London-van der Waals dispersion forces, the Sinanoğlu-Pitzer-McLachlan interaction, are fairly well determined for the adsorption on Ag(111); this has been reviewed elsewhere [2]. The success of the statistical mechanical modelling of the Xe/Ag(111) adsorption [40] has been taken to mean that no large terms have been omitted from the interactions there. For Xe/Pd(100) the observed phenomena are grossly different [3] from the Xe/Ag(111) case; estimates of the contributions of the adsorption dipoles and the McLachlan

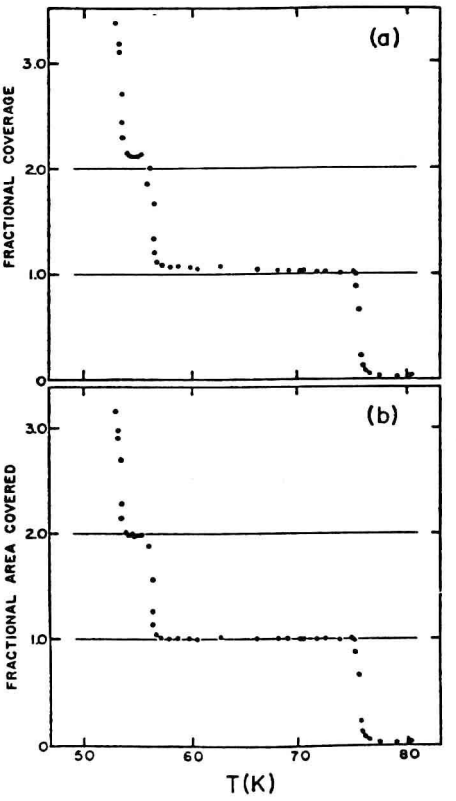


Figure 2. a) Fractional Xe coverage on Ag(111) for a flux of 3D gas at effective pressure $p = 3 \times 10^{-8}$ torr. b) Fractional area, formed by combining the data of (a) with the measured lattice constant of the Xe adlayer, Ref. 5.

interactions do not lead to large enough effects to account for the difference. While one approach has been to argue for the importance of finite geometry effects [43] in this case, it is also plausible that additional substrate-induced processes leading to substantial modification of the overlap interaction of Xe atoms arise because of the larger chemical activity of the palladium substrate. Even if the interaction model is known, the observations of the monolayer solids cover temperature ranges with substantial thermal excitation and the evaluation of the statistical mechanics itself becomes complex.

A relatively simple limit of the statistical mechanics is at low temperatures where a small amplitude oscillation approximation [39] for the atomic motions is accurate except for the light inert gases. This is the quasiharmonic approximation, using the harmonic lattice dynamics; the special-points evaluation of Brillouin zone sums [44] makes it a very rapid calculation. The quasiharmonic approximation has the advantage of including

collective motions of the solid, the normal modes of vibration, and leads to a Debye theory at very low temperatures. However, experience with extending the theory to include anharmonic effects by perturbation theory at intermediate temperatures has been rather discouraging. A surprising but useful result from several studies [45,46] has been that an approximation which treats the anharmonicity in some detail, but largely neglects the correlations is frequently quantitatively useful at intermediate temperatures. This is a version of the Einstein model of a solid, based on the Lennard-Jones and Devonshire cell theory [45], in which the motion of a central atom in the field of its fixed neighbors is calculated exactly without recourse to small amplitude displacement approximations. Although the approximation can be formulated as a variational mean field theory, in practice it has frequently been applied [40,46] without a self-consistent determination of the average cell potential. The accuracy of the approximation was established in calculations for 2D Xenon interacting via Lennard-Jones (12,6) potentials at low temperatures by comparing to the results of the quasiharmonic theory [39] and at high temperatures, approaching melting conditions,comparing to the results of Monte Carlo simulations [46,47]. An application of the cell model for cases such as neon was developed [42]: in place of a classical continuum evaluation of the cell partition function, the partition function was evaluated from the quantum mechanical energy levels for motion in the cell potential. A technical difficulty in developing the numerical methods was eventually traced [42] to the fact that the error-determining step in a matrix formulation of the Schrödinger equation in mathematical 2D is different than in 3D;it is the approximation to a boundary condition at zero separation in 2D.

Table 1

Monolayer Solids

	Ne	Ar	Xe
$\varepsilon(K)^{(a)}$	37	120	230
$r_o(\mathring{A})^a$	3.13	3.82	4.50
Λ^*	0.58	0.19	0.06
L_o/r_o	1.050	1.007	0.9956
E_o/ε	-2.25	-3.01	-3.25
$K_T(\varepsilon/r_o^2)$	0.0303	0.0177	0.0144

[a]Energy and length scales of Lennard-Jones (12,6) potentials.

A summary of properties calculated for Lennard-Jones models of monolayer solids is presented in Table 1. The pair potential for atoms at separation r is

$$\phi(r) = \varepsilon\{(r_o/r)^{12} - 2(r_o/r)^6\} \qquad (2.1)$$

and the de Boer parameter is defined by

$$\Lambda^* = (h/r_o\sqrt{m\varepsilon})2^{1/6}, \qquad (2.2)$$

where h is Planck's constant and m is the atomic mass. The reduced monolayer lattice constant at zero spreading pressure, L_o/r_o, the ground state energy E_o/ε and the dimensionless compressibility are listed there for conventional parameters for Ne, Ar, and Xe. For comparison, the corresponding values for pure classical solids ($\Lambda^*=0$) are $L_o/r_o = 0.97$ in 3D and $L_o/r_o=0.9902$ and $Eo/\varepsilon=-3.382$ in 2D. The 2% expansion in L_o from 3D to 2D, which is purely a consequence of lattice geometry in this calculation, is in fortuitous agreement with the expansion observed for Xe/Ag(111). That expansion is now known [48] to arise from the combination of several partially offsetting 1% effects to the determination of L_o.

The entries for Neon [49] in Table 1 show the effects of large zero-point energy effects. Attempts to develop a perturbation theory of the monolayer solid show the dilation is so large that there are substantial anharmonic effects [50]. The large compressibility, also an effect of the dilated lattice, is associated with a large compression of the monolayer between its condensation and second layer formation. The change in lattice constant is found [49] with various models for Ne/Gr to be 4 to 5%, or double the change for Xe/Ag(111). The magnitude of the lattice constant at bilayer formation was calculated to be close to the measured near-neighbor spacing of 3D Ne at the sublimation curve L_s. Experiments found it to be 1 to 2% smaller than L_s [33,34]; part of the difference is related to uncertainty in the length scale of the 3D pair potential [51]. This discrepancy has some consequence for the understanding of the crystal growth mode of Ne/Gr. The Ne/Gr system has been proposed to follow a Stranski-Krastanov growth mode, with the driving factor being the mismatch in lattice constant between the compressed monolayer and the 3D solid at sublimation [10,16]. According to this argument it is likely that the compressed monolayer solids of D_2/Gr and H_2/Gr also follow this growth mode because they show even larger compressions relative to their 3D solids [52].

There are, however, competing effects which may change the behavior. The monolayer of Xe/Gr at its limit of compression [8] has, at 60 K, a value of L which is 2.5% smaller than L_s; however the bilayer then "springs back" and has an L value close to L_s, a phenomenon of "inverted epitaxy" [53]. This could occur for other strongly compressed layers. Second, the over-compression of the quantum layers is related to their relatively large compressibility; the large compressibility would also lower the energy needed to form dislocation-like lattice defects to heal the lattice toward the bulk structure [9]. These are structural processes which may be difficult to infer without detailed diffraction studies of the few-layer system.

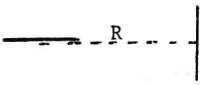
3. Linear Molecules

For the intrinsic inert gas monolayer the atomic packing problem is simple and the structure is the close-packed triangular lattice; there is no other 2D Bravais lattice close in energy to this except for a degenerate limit of the centered rectangular lattice. Even for the double layer, which is a close-packed stack of two triangular lattices, the structure to be studied is readily apparent. At the trilayer, the question of the stacking sequence arises [7]: whether it is the beginning of the hexagonal close-packed or face-centered cubic sequence of the 3D solids. The energies of the two 3D

structures are very close in magnitude and it is conceivable that the external potential provided by the substrate might lead to different initial stacking sequences than the bulk. Some phonon spectra for the trilayers of Ar,Kr, and Xe on Ag(111) are now available from inelastic helium atom scattering [6], but the resolution is not high enough to use the observed dispersion relations to distinguish between the stacking sequences.

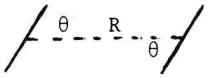
The packing problem for thin layers of small linear molecules is much more complex. In the Pa3 crystal structure of 3D solids of N_2 and of CO_2 [54] the molecules are not flat in the close-packed plane of the solid and the solid consists of 4 sublattices. Under compression the N_2/Gr monolayer may form a pinwheel structure [20] with molecules oriented at angles to the adsorbing plane. However, in most calculations to determine the configuration at monolayer solid condensation, two interpenetrating rectangular lattices of different molecular orientations, a herringbone pattern [21,22], are considered as the most likely structure. The determination of the minimum energy lattice then includes electrostatic interactions of permanent quadrupole moments of the molecules (and the effect of substrate screening charges) and the overlap repulsions and van der Waals attractions among the admolecules [22]. The overlap repulsions lead to angles for the herringbone array which differ from the angle which minimizes the energy of the quadrupoles on opposite sublattices.

For two quadrupoles of moment Q and separation R oriented so that their axes are coplanar with the separation vector the configuration of lowest electrostatic energy Q has the axes perpendicular to each other



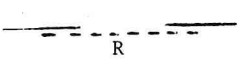
$$\phi_Q = -3Q^2/R^5. \tag{3.1}$$

There is another coplanar configuration with electrostatic energy close to this



$$\phi_Q = -(18/7)Q^2/R^5, \tag{3.2}$$

where the angle θ is the inverse cosine of $\sqrt{3/7}$. The highest energy configuration has



$$\phi_Q = 6Q^2/R^5. \tag{3.3}$$

The fact that Eq.(3.1) and (3.2) are so close in magnitude means that both sets of near neighbors in a planar herringbone lattice can have nearly minimal electrostatic interaction energy [55].

The quadrupolar energies are a major portion of the cohesive energy of 3D solid CO_2 [56]. Thus, the experimental proposal [19] that CO_2 does not wet graphite at low temperatures, even to the extent of forming a monolayer solid,

stimulated a model calculation [22] of the ground state energy of the monolayer solid including the electrostatic screening response of the substrate. As in the evaluation of the substrate-mediated dispersion energies [2], ideal screening response to external charges was used at very small separations, where it clearly becomes a rough approximation to the substrate response.The result of the calculations, for a two-sublattice model with the CO_2 lying in the adsorbing plane, was that the ground state solid was likely to be incommensurate with the graphite lattice; this differed from a proposed registry structure inferred from the nominal coverage in the experiment. The calculation showed that the substrate screening of the molecular quadrupole moments had a large effect in the ground state energy and that it was marginal whether the model gave wetting. Both these results showed that to make progress in modelling the CO_2/Gr system more knowledge of the holding potential and of its dependence on the angle of the CO_2 axis to the surface normal were needed.

The focus of the model calculation [22] for CO_2/Gr was on the screening response of the substrate and its contribution to the electrostatic portion of the adlayer energy. However there is a second perspective [14] which also suggests the difficulty of a smooth growth of the adsorbed film: the bulk solid in this orientation has close-packed planes where the molecules are at angles relative to the plane [54]. It is difficult to extend smoothly from the likely first layer packing to this type of geometry.

The discussions of bilayer formation in Sec.2 and of the CO_2 layer here both are based on pictures of thin films with well-defined layer structure. In the modelling of the bilayer films at intermediate temperatures a failure of the approximations came [37] when the perpendicular motions of second layer atoms became large and led to poor definition of the second layer. The fact that the CO_2 monolayer film wets Gr at temperatures above 104 K but not at lower temperatures [19] appears difficult to understand in the context of the layered solid picture. The monolayer solid becomes favorable in chemical potential relative to the bulk solid at a high enough temperature, which means that entropy plays a major role. For the monolayer solid to have higher entropy than the 3D solid probably requires significant motions of the adsorbate out of the monolayer plane.

4. Registry Adlayers

The modulation phenomena in monolayer solids adsorbed on strongly corrugated substrate surfaces reflect the competing periodicities of the intrinsic adlayer and of the substrate. In this context one makes contact with general concepts of frustrated interactions and with specific models of the nonlinear response of idealized models such as the Frenkel-Kontorova, Frank-van der Merwe, one-dimensional chain in a periodic potential [57,58,59]. The most extensively studied monolayers showing these phenomena are triangular adlayer lattices on the basal plane surface of graphite [60]. The theoretical analysis has been difficult and complicated because some of the significant modulation patterns are two-dimensional intersecting arrays of misfit dislocations or domain walls [61,62]. However, there are systems where the substrate potential has approximately rectangular symmetry and which appear to be simpler to treat [26]: inert gases on the (110) face of face-centered cubic metals. There is not yet a great deal of data on these systems [23,24,25,63], but the available information has been used [26] to make some estimates of the corrugation of the one-atom holding potential and to identify features in the data which are

difficult to understand or surprising in the context of simple models of the adlayer response.

The corrugation of the holding potential for a planar substrate surface is expressed in terms of the Fourier decomposition of the holding potential [64]:

$$V(r,z) = V_o(z) + \Sigma_{g(\neq 0)} V_g(z) e^{ig \cdot r}; \qquad (4.1)$$

the Cartesian coordinate axes have the z-component perpendicular to the surface and the vector r (with x and y components) parallel to the surface plane. The vectors g are the reciprocal lattice vectors of the substrate surface plane. For model holding potentials formed by summing the interactions of adatom-substrate atom pairs [64], the Fourier amplitudes V_g decrease in magnitude rapidly with increasing magnitude of g for weakly corrugated surfaces. Measurements of the scattering of helium atoms from Pd(110) have shown the first few amplitudes decrease rapidly [65].

When the surface lattice of the substrate has a different symmetry, such as rectangular or centered rectangular, than the triangular lattice of an intrinsic monolayer of an inert gas, the description of registry must be generalized from the case of the triangular adlayer on triangular surface [4]. Also, a rectangular surface lattice may drive distortions of the adlayer lattice to a centered rectangular lattice or even to an oblique lattice. Simple registry in these cases arises when elements of the reciprocal lattice of the adlayer coincide with some elements of the reciprocal lattice g of the substrate surface [4]. Coincidence with leading surface reciprocal lattice vectors may also occur after small adlayer distortions to a lattice with more than one atom per unit cell [66], as perhaps is the case for Ne/Gr at very low temperatures [34]. However the net lowering of the adlayer energy for optimized positions in the larger unit cell is expected to be smaller [66,67] than energies arising directly from the leading terms in Eq. (4.1). Detailed analysis has so far only been performed for the case of the adlayer with one atom per unit cell. Also, if the uniaxial registry persists through the monolayer regime, the formation of the bilayer may occur at a chemical potential very close to the bulk value and the structural misfit may make it difficult to achieve an extended layer-by-layer growth. This possibility was examined in a model calculation [27] for uniaxially registered Xe/Cu(110): the calculated bilayer formation was very close to the bulk condensation.

We now discuss model calculations [26] for planar centered rectangular adlayers on rectangular adsorbing lattices. As coordinates of the fcc(110) surface take the x-axis to be along the [001] direction and the y-axis along the [110] substrate is ℓ, the distance between nearest neighbors at the (110) surface is $\ell\sqrt{2}$ in the [001] direction and ℓ in the [110] direction. There are close-packed troughs on the surface running parallel to the y-axis. Uniaxially registered lattices where the atoms of a centered rectangular adlayer reside in these troughs are observed for Xe/Ag(110) [23], Xe/Cu(110) [23,24], and Kr/Cu(110)[24,25]. The lateral interactions of inert gas atoms such as Xe and Kr in island-forming systems are fairly well known [2,8,38]. Thus the occurrence of the registry lattices can be used to make estimates of the amplitudes of the corrugation potential in a truncated series corresponding to Eq. (4.1):

$$V(r,zo)=Vo + 2\ V_1\ \cos(2\pi\ x/\ell\sqrt{2}) +2\ V_2\ \cos(2\pi\ y/\ell). \qquad (4.2)$$

The amplitudes V_1 and V_2 must be large enough that it is energetically favorable to distort the adlayer lattice from the intrinsic uniform triangular lattice to the (uniaxially) registered structures. A first estimate [26],which provides a lower bound on the critical potential amplitude, is to compare the value of the lateral potential energy in the two structures. Indeed, although this comparison does not explicitly treat the energy of modulated adlayer lattices of small misfit relative to the registry lattice, it agrees with the result of the more detailed calculation to about 20%.

The detailed calculation [26] is a version of the Frank-van der Merwe calculation for a harmonic linear chain in an external sinusoidal potential [57,60]. The average centered rectangular lattice is modulated with harmonics of the misfit wave vector (the smallest reciprocal lattice vector difference between adlayer and surface lattice). The dispersion relation of the adlayer normal modes, for a Lennard-Jones (12,6) pair potential between adatoms, is included and the interaction energy with the periodic substrate potential is evaluated as a continuum average, which omits the pinning potential [66] for dislocations on a discrete surface. The amplitudes of the positional modulations are adjusted to minimize the total energy [59]. Anharmonic effects enter in two partially offsetting ways. First, the harmonic elastic constants for inert gas adlayers are very rapid functions of the lattice constant, as noted by Venables [61]. Second, for the rather dilated lattices which occur for the C(2X2) lattice of Xe/Cu(110) and for Xe/Ag(110) and for the compressed (along [001]) spacings of Xe/Cu(110), the nonlinear response of the adlayer is important in limiting the size of the modulation amplitudes. The sort of pathology which can occur if the anharmonic response is not included is shown in model calculations [26] to determine the value of V_2 needed to stabiize the C(2X2) lattice of Xe/Cu(110) relative to the optimized uniaxial registry lattice (registry only along the x-axis).The dilation in the [110] direction relative to the optimized uniaxial lattice is 6% to 10%, depending on the lateral interaction model; it is so large that the harmonic lattice constants become so small for displacments along the [110] direction that states of finite misfit occur where essentially all the adatoms are in registry positions and the misfit is taken up in a small fraction of an interatomic spacing. That is, nearly the full registry energy is available at small finite misfit because the domain walls are very narrow; the cubic and quartic anharmonic perturbation theory terms both restore the situation of broader domain walls.

Another method to estimate the critical values of V_1 and V_2 to stabilize the registry structures is [26] to use the results of the continuum Frank-van der Merwe theory [57] for a linear harmonic chain, with the adlayer elastic constant as a parameter. As just noted, when the registry lattice is quite dilated relative to the intrinsic triangular lattice the harmonic elasticconstants are small; inclusion of anharmonic effects increases the effective elastic constants. Also, if the registry structure is strongly compressed the stability of the registry structure requires a more detailed comparison of lattices at distinctly different lattice constants, since the onset of the registry as a function of V_1 can be [26] a "first order

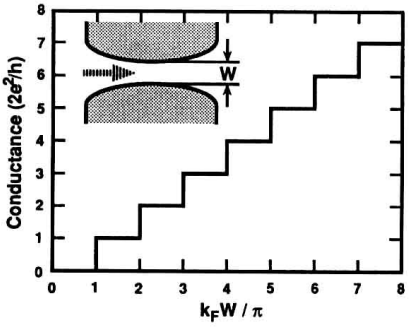


Fig. 11 Conductance across a narrow constriction versus electron wavelength in an ideal case. The inset illustrates an ideal quantum point contact in which the boundary varies much more slowly than the electron wavelength.

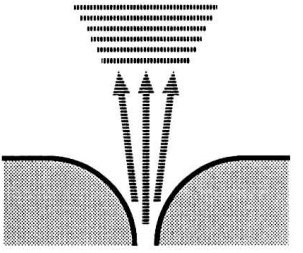


Fig. 12 Collimation of electron beam injected by a quantum point contact. Because of the large rounding of the corners of the boundary, the electron waves are collimated in the forward direction.

ing the length scale of the order of the screening length or the electron wavelength. Therefore, effects of rough boundaries are usually less important than one might expect except in some special systems where boundary roughness is introduced intentionally. A strong boundary roughness gives rise to a peculiar positive magnetoresistance observed experimentally [35] and analyzed theoretically [36] in quantum wires fabricated at GaAs/AlGaAs heterostructures. This topics is treated in Part IV in this volume.

One of the most typical phenomena observed in the ballistic regime is the conductance quantization across a quantum point contact [37-39]. By the metallic gate fabricated on top of the two dimensional system at a GaAs/AlGaAs heterostructure and by a negative bias voltage we can create a narrow path connecting two spatially separated 2D electron systems. The conductance across this quantum point contact was observed to be quantized into integer multiples of $e^2/\pi\hbar$ as shown in Fig. 11.

The electron wave emitted from a quantum point contact is collimated in such a way that the electron propagates mainly in one direction instead of being emitted as a point source from which electrons propagate as a spherical wave. This collimation is a result of a considerable rounding of the corner of the confining potential as illustrated in Fig. 12 and has been observed in the magnetic-field dependence of the conductance across series of point contacts [40] and also in magnetic focusing experiments [41]. The nature of this point contact can be used as electron emitters and collectors in ballistic quantum structures (electron optics) [42]. Interference of electron waves passing through regions with different electron concentrations has also been observed and used for the determination of the strength of electron-electron scattering of 2D electrons both as function of energy and temperature [43]. Nonlinear conduction has also been a subje of recent study but is not included in this volume.

Usually, the transport coefficients in quantum wires are measured using a crossed-wires geometry. Various interesting phenomena arising from ballistic transmission across junctions of quantum wires have been observed. One most typical example is the anomalies in the low-field Hall effect such as the quenching and last plateau [44-46]. In weak magnetic fields, the Hall resistance has been observed to be much smaller than classical $\rho_H = H/nec$ (quenching) but increases rapidly and stays almost independent of the field (last plateau) beyond a certain magnetic field as shown in Fig. 13.