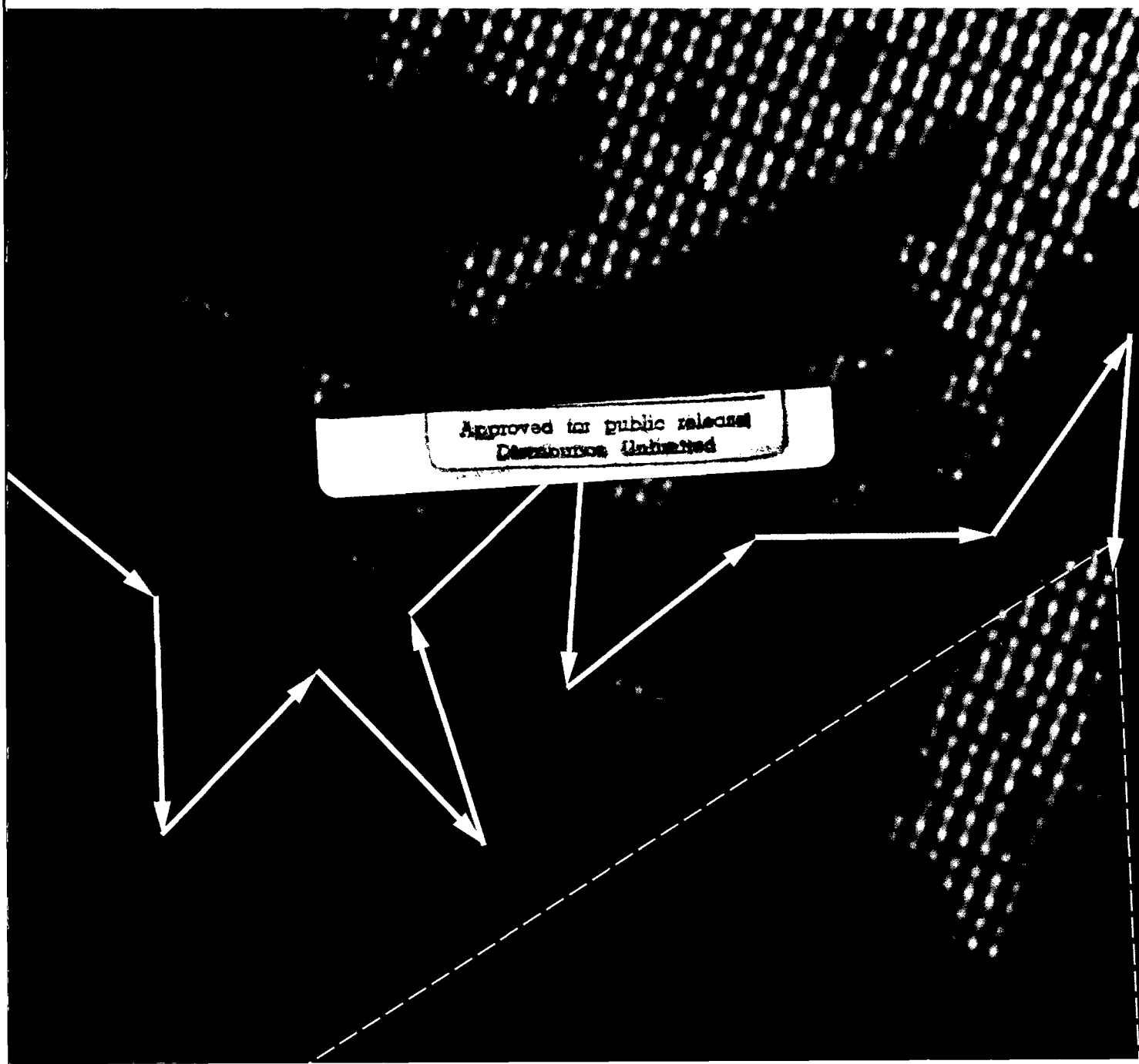


SURFACE DIFFUSION: Atomistic and Collective Processes

***NATO Advanced Study Institute
Rhodes, Greece — August 26 - September 6, 1996***

DTIC QUALITY INSPECTED 3



NATO Advanced Study Institute Surface Diffusion: Atomistic and Collective Processes Conference Program

August 26-September 6, 1996
Olympic Palace Hotel
Rhodes, Greece

The 50-minute talks will be 45 minutes talk with 5 minutes for questions; 25-minute talks will be 22 and 3, and the 12-minute talks will be 10 and 2.

Sunday, August 25, 1996

19:30-21:30 Welcoming Party and Pre-registration at the Olympic Palace Hotel

Monday, August 26, 1996

8:30 Registration
8:45 Opening and Welcoming Remarks

Morning Session

Chairperson: G. Comsa

9:00 **Lecture:** R. Gomer, University of Chicago, *Recent results from the fluctuation method: I*
9:50 **Lecture:** D. A. King, Cambridge University, *Concentration profile measurements of surface diffusion*
10:40 Coffee Break

Chairperson: D. A. King

11:10 **Lecture:** H. Pfner, Universitat Hannover, *Thermal fluctuations in equilibrium and their modifications by surface defects*
12:00 **Lecture:** B. Cooper, Cornell University, *Stability and decay of nanoscale surface features*
12:50 Lunch and Discussions

Evening Session

Chairperson: G. Ehrlich

17:00 **Lecture:** S.-C. Ying, Brown University, *Study of surface diffusion through Langevin dynamics*
17:50 **Lecture:** P. Toennies, Max-Planck-Institut für Strömungsforschung, *Quasielastic helium atom scattering studies of microscopic surface diffusion: 1. Method and theory*
18:40 **Lecture:** K. Fichtorn, Penn State University, *The diffusion of large, adsorbed molecules on metal surfaces*
19:30 End of Session

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DTIC QUALITY INSPECTED 3

Tuesday, August 27, 1996

Morning Session

Chairperson: R. Gomer

9:00

Lecture: T. Tsong, Academia Sinica, *Diffusion of single atoms and small atom clusters on terraces and stepped surfaces: I*

9:50

Lecture: J. Villain, Centre d'Etudes Nucléaires de Grenoble, *Kinetic coefficients in a system far from equilibrium*

10:40

Coffee Break

Chairperson: P. J. Feibelman

11:10

Lecture: Harald Brune, Ecole Polytechnique Federale Lausanne, *Kinetics of metal epitaxy*

12:00

Lecture: C. Ratsch, Fritz-Haber-Institut der Max-Planck-Gesellschaft, *Density-functional theory of diffusion and growth*

12:50

Lunch and Discussions

Evening Session

17:00

Poster Session I

19:30

End of Session

Wednesday, August 28, 1996

Morning Session

Chairperson: J. P. Toennies

9:00 **Lecture:** G. Ehrlich, University of Illinois at Urbana—
Champaign, *Atomic jump processes in crystal growth: Direct observations and kinetic consequences*

9:50 **Lecture:** P. Feibelman, Sandia National Laboratory, *A chemical view of bonding and diffusion at surfaces: I*

10:40 Coffee Break

Chairperson: J. Villain

11:10 **Lecture:** J. Frenken, Leiden University, *Hoppa! Dances with kinks*

12:00 **Lecture:** G. Rosenfeld, IGV, *Diffusion and stability of large clusters on crystal surfaces*

12:50 Lunch and Discussions

Evening Session

Chairperson: S.-C. Ying

17:00 **Lecture:** P. Toennies, Max-Planck-Institut für Strömungsforschung, *Quasielastic helium atom scattering studies of microscopic surface diffusion: Experimental Results and Their Interpretation*

17:50 **Lecture:** D. A. King, Cambridge University, *Reaction kinetics and spatiotemporal oscillations*

18:40 **Lecture:** U. Kuerpick, Kansas State University, *The role of vibrations in adatom diffusion*

19:30 End of Session

Thursday, August 29, 1996

Morning Session

Chairperson: H. Metiu

9:00 **Lecture:** G. Comsa, IGV-KFA-Forschungszentrum,
Surface diffusion and film growth: I

9:50 **Lecture:** G. Comsa, IGV-KFA-Forschungszentrum,
Surface diffusion and film growth: II

10:40 Coffee Break

Chairperson: B. Cooper

11:10 **Lecture:** J. Evans, Ames Laboratory, *Submonolayer
nucleation and growth, and transition to multilayer kinetic
roughening during metal (100) homoepitaxy*

12:00 **Lecture:** Z. Zhang, Oak Ridge National Laboratory,
Dynamics of ad-dimers at surfaces

12:50 Lunch and Discussions

Evening Session

Chairperson: T. Tsong

17:00 **Lecture:** H. Metiu, University of California—Santa
Barbara, *Beating the Time Scale in Computer Simulation of
growth: From atom motion to coarsening*

17:50 **Lecture:** G. Ehrlich, University of Illinois at Urbana—
Champaign, *Surface diffusion of metal atoms and clusters
directly observed*

18:40 **Lecture:** M. Horn-von Hoegen, Universität Hannover,
*Surfactant mediated heteroepitaxy interplay of diffusion,
strain relief and surface morphology*

19:30 End of Session

Friday, August 30, 1996

Morning Session

Chairperson: H. Pfnuer

- 9:00 **Lecture:** M. Henzler, Universität Hannover, *LEED investigation of surface processes I*
- 9:50 **Lecture:** P. Cohen, University of Minnesota, *Microscopic mechanisms of surface segregation: Sn doped GaAs (100)*
- 10:40 Coffee Break

Chairperson: J. Frenken

- 11:10 **Lecture:** A. Naumovets, Academy of Sciences of Ukraine, *Surface diffusion and phase transitions in atomic overlayers: I*
- 12:00 **Lecture:** E. Conrad, Georgia Tech, *Entropic step doubling on (110) vicinal tungsten surfaces*
- 12:50 Lunch and Discussions

Evening Session

Chairperson: Z. Zhang

- 17:00 **Lecture:** M. C. Tringides, Ames Laboratory & Iowa State University, *Adsorbate-adsorbate interactions and surface diffusion*
- 17:50 **Lecture:** M. Zinke-Allmang, University of Western Ontario, *Role of surface diffusion during late stage clustering*
- 18:40 **Lecture:** A. Andriotis, The University of Crete & FORTH, *The interaction of Ni and Si atoms with the Si(110) surface*
- Lecture:** M. Asscher, Hebrew University, *Optical studies of surface diffusion: SHG diffraction experiments and simulations*
- 19:30 End of Session

Monday, September 2, 1996

Morning Session

Chairperson: M. Scheffler

- 9:00 **Lecture:** R. J. Behm, Abteilung Oberflächenchemie und Katalyse, *Nucleation and growth in epitaxy—beyond simple, site independent hopping diffusion, I*
- 9:50 **Lecture:** J. Reutt-Robey, University of Maryland, *Mass transfer in surface chemical processes: Adsorption, faceting, and reaction on Ag(110)*
- 10:40 Coffee Break

Chairperson: R. J. Behm

- 11:10 **Lecture:** T. Tsong, Academia Sinica, *Diffusion of single atoms and small atom clusters on terraces and stepped surfaces: II*
- 12:00 **Lecture:** P. Ruggerone, Fritz Haber Institut, *Microscopic processes behind homoepitaxial growth of metallic systems*
- 12:50 Lunch and Discussions

Evening Session

Chairperson: H. Brune

- 17:00 **Lecture:** M. Scheffler, Fritz-Haber-Institut der Max-Planck-Gesellschaft, *Self-ordering of nano-structures on GaAs surfaces*
- 17:50 **Lecture:** C. Teichert, Max-Planck-Institut für Mikrostruktur-physik, *Stress-driven morphological changes of SiGe Films grown on vicinal Si(001) substrates*
- 18:40 End of Session

Tuesday, September 3, 1996

Morning Session

Chairperson: M. Henzler

- 9:00 **Lecture:** R. Gomer, University of Chicago, *Recent results from the fluctuation method: II*
- 9:50 **Lecture:** H. Metiu, University of California—Santa Barbara, *The equilibrium shape and the "vapor" pressure of an island*
- 10:40 Coffee Break

Chairperson: G. Rosenfeld

- 11:10 **Lecture:** M. Henzler, Universität Hannover, *LEED investigation of surface processes II*
- 12:00 **Lecture:** S. Stoyanov, Bulgarian Academy of Sciences, *Diffusion and electromigration of Si adatoms on vicinal Si surfaces—formation and relaxation of bunches of steps*
- 12:50 Lunch and Discussions

Evening Session

Poster Session

- 17:00 **Poster Session II**
- 19:30 End of Session

Wednesday, September 4, 1996

Morning Session

Chairperson: M. Horn-von Hogen

- 9:00 **Lecture:** J. Villain, Centre d'Etudes Nucléaires de Grenoble, *Epitaxial clusters: Equilibrium properties vs. kinetics*
- 9:50 **Lecture:** D. Kandel, Weizmann Institute of Science, *Effects of surfactants on surface diffusion*
- 10:40 Coffee Break

Chairperson: A. G. Naumovets

- 11:10 **Lecture:** R. J. Behm, Abteilung Oberflächenchemie und Katalyse, *Nucleation and growth in epitaxy—beyond simple, site independent hopping diffusion: II*
- 12:00 **Lecture:** P. Feibelman, Sandia National Laboratory, *A chemical view of bonding and diffusion at surfaces: II*
- 12:50 Lunch and Discussions

Evening Session

Chairperson: P. Cohen

- 17:00 **Lecture:** S.-C. Ying, Brown University, *Study of surface diffusion through Langevin dynamics*
- 17:50 **Lecture:** I. Markov, Bulgarian Academy of Sciences, *Surface energetics from nucleation data analysis in homoepitaxy*
- 18:15 **Lecture:** X. Xiao, Hong Kong University of Science & Technology, *Impurity effects on surface diffusion: S, O, K on CO/Ni(110)*
- 18:40 End of Session

Thursday, September 5, 1996

Morning Session

Chairperson: C. Uebing

9:00 **Lecture:** A. Naumovets, Academy of Sciences of Ukraine, *Surface diffusion and phase transitions in atomic overlayers: II*

9:50 **Lecture:** X. Zhu, University of California—Davis, *Recent results of hydrogen diffusion on Ni(111) at low temperatures: Searching for the evidence of quantum tunneling diffusion of hydrogen on Ni(111)*

10:40 Coffee Break

Chairperson: S. Stoyanov

11:10 **Lecture:** C. Uebing, Physikalische Chemie, *Monte Carlo simulation of surface diffusion on homogeneous and heterogenous surfaces*

12:00 **Lecture:** J. Wollschlaedger, University of Hannover, *Epitaxial growth of Mg/Ag(100): Transition from complete condensation to adsorption-desorption equilibrium*

12:50 Lunch and Discussions

Evening Session

Chairperson: C. Tiechert

17:00 **Lecture:** Gomez-Rodriguez, Universidad Autonoma de Madrid, *Scanning tunneling microscopy study of single Pb atom diffusion on Si(111) 7×7 and Si(111) 5×5 surfaces*

17:25 **Lecture:** G. Vidali, Syracuse University, *Investigations of adsorption, recombination and desorption of H on low temperature surfaces of bare and ice-covered silicates*

17:50 **Lecture:** M. Jalochoowski, Institute of Physics UMCS, *Low-temperature epitaxial growth of thin metal films: in situ electrical resistivity study*

18:40 End of Session

Friday, September 6, 1996

Morning Session

Chairperson: J. Wollschlaedger

- 9:00 **Lecture:** M. Altman, Hong Kong University of Science and Technology, *Impact of step edge barriers in step flow growth studied by LEEM*
- 9:25 **Lecture:** M. Zaluska-Kotur, Polish Academy of Sciences and College of Science, *Diffusion coefficient for interacting lattice gases—random potential approach*
- 9:50 **Lecture:** Marc Langelaar, Groningen University, *Atomic mobility of Ag and Fe on the Ag(100) surface*
- 10:15 **Lecture:** I. Vattulinen, University of Helsinki, *Studies of surface diffusion under non-equilibrium conditions*
- 10:40 Coffee Break

Chairperson: C. Ratsch

- 11:10 **Lecture:** T. Linderoth, University of Aarhus, *Real-time imaging of the diffusion, nucleation, and growth of Pt on Pt(110)/K. Morgenstern, University of Aarhus, *Adatom and vacancy island decay at variable temperatures**
- 11:35 **Lecture:** P. Jensen, CNRS, *Diffusion of large clusters: Experiments and simulations*
- 12:00 **Lecture:** R. Kutner, Warsaw University, *Transport coefficients in a transient state on a one-dimensional lattice*
- 12:25 **Lecture:** H. Dobbs, Imperial College, *Theory of coherent island growth*
- 12:50 Concluding Remarks

**NATO Advanced Study Institute
Surface Diffusion:
Atomistic and Collective Processes
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**August 26-September 6, 1996
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Monday, August 26, 1996

9:00

Lecture: R. Gomer, University of Chicago, *Recent results from the fluctuation method: I*

Recent Results from the Fluctuation Method: I. R. GOMER, University of Chicago. - - - Methods for determining diffusion coefficients from adsorbate density fluctuation autocorrelation functions will be presented and discussed with emphasis on the field emission technique. The basic theory of the methods is reviewed briefly and experimental implementations as well as problems are discussed.

9:50

Lecture: D. A. King, Cambridge University, *Concentration profile measurements of surface diffusion*

11:10

Lecture: H. Pfnuer, Universitat Hannover, *Thermal fluctuations in equilibrium and their modifications by surface defects*

Thermal Fluctuations in Equilibrium and Their Modifications by Surface Defects.
H. PFNUER, Institut für Festkörperphysik, Universität Hannover, Appelstrasse 2, Hannover D-30167, Germany. - - - Fluctuations in thermal equilibrium are much more pronounced in two than in three dimensions, leading to a widespread occurrence of continuous phase transitions in 2D. Their correlations and relative magnitudes can be quantified by studies of critical scattering close to continuous phase transition, e.g., by using low energy electrons. Impurities and other defects modify the fluctuations and their correlations, but may also change the character of the phase transition completely.

As model systems for corresponding experimental studies in 2D, we chose strongly chemisorbed atomic adsorbates on close packed transition metal surfaces. For pure systems, the power law behavior expected theoretically for continuous phase transitions in various universality classes has been also found in experiment, with surprisingly small corrections to scaling even far away from the critical temperatures.

Effects of various types of defects will also be presented. It turns out that even different isotopes in a system like atomic H on Ni(111) may act as defects, changing the order-disorder phase transition of a (2×2) ordered layer from second to first order, and leading to a tendency to phase separate close to T_c . Oxygen impurities, on the other hand, do not destroy the continuous phase transition, but modify the critical exponents. A similar effect occurs, if the order of the adsorbate couples across steps. These results are discussed in the framework of random disorder.

12:00

Lecture: B. Cooper, Cornell University, *Stability and decay of nanoscale surface features*

Stability and Decay of Nanoscale Surface Features. B. H. COOPER, J. G. McLean, D. R. Peale, B. Krishnamachari, and J. P. Sethna, Dept. of Physics - Clark Hall, Cornell University, Ithaca, New York 14853 USA. - - - We have studied general issues regarding the stability of nanoscale surface features, e.g., pits and islands one or a few atomic layers in height. Such features are formed as intermediate structures during growth, etching, and sputtering. Results will be presented showing the decay of such features under different experimental conditions. Using a simple thermodynamic model, the relative importance of different microscopic processes in controlling the decay and/or stability can be examined. This model is similar to earlier ones derived for studying nucleation and growth. The driving force for the decay is the Gibbs-Thomson effect, i.e., the enhancement of the equilibrium vapor pressure at curved edges. In order to test the validity of using the Gibbs-Thomson relation at small island sizes we have developed a Monte Carlo solid-on-solid simulation using simple bond-counting energetics. We have computed the vapor pressure of adatoms in equilibrium with islands of different radii, down to very small system sizes. We find that the Gibbs-Thomson law qualitatively reproduces these results, but disagrees at small island radii and high temperatures. We find quantitative agreement when we use an equation of state more accurate than the ideal gas law to derive a modified Gibbs-Thomson relation. Simulations of island and pit decay will be presented in which we examine the sensitivity of the decay rate to rates of different microscopic processes.

17:00

Lecture: S.-C. Ying, Brown University, *Study of surface diffusion through Langevin dynamics*

Study of Surface Diffusion Through Langevin Dynamics Outline of Two Lectures:

I. S. C. YING, Department of Physics, Brown University, Providence, Rhode Island 02912. - - - We present in these two lectures the theoretical investigation of adatom diffusion based on Langevin dynamics. In the first lecture, we derive a Generalized Langevin Equation from a microscopic Hamiltonian and discuss its application to the study of surface diffusion. In particular, we focus on how the diffusion constant depends on the friction parameter characterizing the non-adiabatic coupling of the adatom to the substrate excitations. We will discuss such topics as the validity of the transition state theory, occurrences of long jumps and memory effects in determining the prefactor and the barrier for surface diffusion. In the second lecture, we discuss the application of the formalism to two specific systems. The first system is adsorption on W(100) which undergoes a displacive phase transition. We show that the friction and hence the diffusion constant exhibits anomalous temperature dependence near the transition due to critical fluctuations. The second system is Na/Cu(001) for which there are extensive data from recent Helium Atom scattering experiments. We will demonstrate that through a careful analysis of the extensive set of data, the entire potential energy surface of the adsorption system (PES) as well as the friction can be determined. This yields a complete information for the adatom dynamics beyond the simple determination of the diffusion constant.

Tuesday, August 27, 1996

9:00

Lecture: T. Tsong, Academia Sinica, *Diffusion of single atoms and small atom clusters on terraces and stepped surfaces: I*

Diffusion of Single Atoms and Small Atom Clusters on Terraces and Stepped Surfaces: I. T. T. TSONG, Institute of Physics, Academia Sinica, Taipei, Taiwan 11529 ROC. - - - Using field ion microscope and scanning tunneling microscope, it is possible to study the diffusion behavior of single atoms and small atomic clusters on flat terraces and stepped surfaces of metals and semiconductors. I will discuss the basic principles and methods of these studies emphasizing our recent studies on stepped surfaces. Diffusion behavior of single atoms and small atom clusters at lattice steps has a great effect on the surface structure of epitaxial films.

9:50

Lecture: J. Villain, Centre d'Etudes Nucléaires de Grenoble, *Kinetic coefficients in a system far from equilibrium*

Epitaxial Clusters: Equilibrium Properties vs Kinetics, Christophe Duport¹, Catherine Priester², J. VILLAIN¹, ¹CEA, D'epartement de Recherche Fondamentale sur la Matière Condensée, SPMM/MP, 38054 Grenoble Cedex 9, France; ²IEMN, D'epartement ISEN, Av. Poincaré BP 69 F-59652 VILLENEUVE D' ASCQ CEDEX France - - -The size distribution of epitaxial islands deposited on a substrate which has a significantly lower lattice parameter is of interest for the realization of quantum dots. A typical example is InAs/GaAs(001), with 7% misfit. The size is certainly diffusion limited, but the shape of each island, at high enough temperature, is the equilibrium shape which corresponds to the island volume at the time of interest. If this volume is low enough, the equilibrium shape is a platelet of thickness 1 monolayer. Now, if the islands are constrained to be 1 monolayer thick, the equilibrium size at fixed coverage is finite, so that, at least at constant coverage (i.e., in the absence of a beam) the radius does not grow in contrast with the Lifshitz-Slyozov theory. The equilibrium platelet size, and the transition to three-dimensional pyramids when the size increases, is studied in the frame of a simple theory and compared with numerical and experimental results for binary semiconductors. There agreement is but qualitative, while certain quantitative features are presumably related to the surface peculiarities of binary semiconductors such as reconstruction.

11:10

Lecture: Harald Brune, Ecole Polytechnique Federale
Lausanne, *Kinetics of metal epitaxy*

Kinetics of Metal Epitaxy. H. BRUNE, IPE, Ecole Polytechnique Federale Lausanne, PHB-Ecublens, CH-1015 Lausanne. - - - The two most important kinetic parameters in epitaxial growth are the energy barriers for terrace- and step-down diffusion. A general concept is shown how to measure these barriers with high accuracy. It relies on the application of mean-field nucleation theory to variable temperature STM data. The validity and limits of this concept will be investigated by comparison of experiment to self-consistent mean-field equations and kinetic Monte-Carlo simulations. It is observed that strain has a pronounced influence on surface diffusion which implies in general a strong layer dependence of growth kinetics for heteroepitaxial systems. The patterns that evolve during low temperature deposition experiments bear detailed information on the atomic diffusion processes involved at the island edge. The relationship between edge-diffusion and the resulting island shape will be analyzed in the case of dendritic growth on trigonal substrates.

12:00

Lecture: C. Ratsch, Fritz-Haber-Institut der Max-Planck-Gesellschaft, *Density-functional theory of diffusion and growth*

Density-Functional Theory of Diffusion and Growth. C. RATSCH*, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin. - - - An introduction to density-functional theory calculations and its application to surface structures will be given. Using this theory we compute the surface diffusion barrier for Pt on Pt(111), Ag on Pt(111), Ag on one monolayer Ag on Pt(111), and Ag on Ag(111). The diffusion barrier for Ag on Ag(111) is studied as a function of lattice mismatch. The step formation energies for Pt(111) are computed and the equilibrium shape of Pt islands is predicted. Additionally, we discuss the reconstruction of the second Ag monolayer on Pt(111) where domains with atoms in the fcc-sites and domains with atoms in the hcp-sites alternate. Our calculations explain why this strain driven reconstruction does occur only after two Ag layers have been deposited.

* Work done in collaboration with G. Boisvert and M. Scheffler.

Wednesday, August 28, 1996

9:00

Lecture: G. Ehrlich, University of Illinois at Urbana—
Champaign, *Atomic jump processes in crystal growth:*
Direct observations and kinetic consequences

Atomic Jump Processes in Crystal Growth - Direct Observations and Kinetic Consequences. G. EHRLICH, Materials Research Laboratory, University of Illinois at Urbana-Champaign, 1304 W. Springfield Ave., Urbana, IL 61801. - - -The behavior of individual metal atoms at metal clusters is believed to play a vital role in the growth of crystals. In some instances, it has been possible to characterize this behavior directly using the field ion microscope. Of particular interest are observations of atoms at lattice steps, which provide information about step-edge barriers. These are briefly reviewed, and reveal behavior not always in keeping with traditional views of crystal growth. The kinetic consequences of different types of step-edge barriers are developed and compared with predictions about Schwoebel barriers.

9:50

Lecture: P. Feibelman, Sandia National Laboratory, A
chemical view of bonding and diffusion at surfaces: I

A Chemical View of Bonding and Diffusion at Metal Surfaces: I. P. J. FEIBELMAN, Sandia National Laboratory, Albuquerque, NM 87185-1413. - - -
Despite the delocalized nature of electrons in metals, elementary chemical ideas, including coordination, valence-saturation and directional bonding, are indispensable guides to the systematics of adatom-metal potential energy surfaces. Drawing from first principles total energy calculations, as well as atomic resolution microscopy data, I will illustrate the application of "chemical thinking" in the (often predictive!) analysis of representative examples. I will discuss the promotion-hybridization view of surface structure and bonding, and show its relevance to materials stability in recent work on "liquid metal embrittlement." I will review the "chemistry" of cluster diffusion and concerted substitution, and explore the systematics of adatom binding near surface defects.

Work supported by the U.S. Department of Energy under contract DE-AC04-94AL85000.

11:10

Lecture: J. Frenken, Leiden University, *Hoppa! Dances with kinks*

Hoppa! Dances with Kinks. J. W. M. FRENKEN^{a,b}, M. S. Hoogeman^a, M. F. Chang^a, M. A. J. Klik^a, and D. C. Schloesser^c, ^aFOM-Institute for Atomic and Molecular Physics, Amsterdam, The Netherlands, ^bKamerlingh Onnes Laboratory, Leiden University, NL, ^cpresent address: Kernforschungszentrum Juelich, Germany. - - - Mass transport on surfaces often proceeds via the fluctuations of monoatomic steps. In these fluctuations, kinks play an important role. In this talk, we present variable-temperature STM observations that provide detailed insight in several aspects of kink dynamics on metal surfaces and their relation with the step motion. We use STM movies to 'see' the spontaneous creation and annihilation of kinks. From the kink statistics we determine the kink formation energy. The motion of the kinks yields the activation energy for the ejection of a single atom from the kink site, either onto a neighboring terrace, or to a location along the step. From correlations in the positions of neighboring kinks, we derive their interactions and from correlations in their motion we get additional information on the kink diffusion mechanism.

You can see our kinks dance at <http://www.amolf.nl/external/wwwlab/general/home.html>.

12:00

Lecture: G. Rosenfeld, IGV, *Diffusion and stability of large clusters on crystal surfaces*

Diffusion and Stability of Large Clusters on Crystal Surfaces.

G. ROSENFELD, IGV, KFA Juelich, D-52425 Juelich, Germany. - - - The mobility and stability of large clusters (consisting of hundreds to thousands of atoms is discussed). Clusters of this size can diffuse across a surface as a result of single atom diffusion events which rearrange the atoms at the cluster boundary causing a center-of-mass shift of the cluster. Depending on the dominant atomic diffusion process (i.e., diffusion along the cluster edge, or evaporation from and re-condensation at the cluster boundary) different scaling properties are found for the cluster diffusion constant as a function of cluster size. Therefore, the atomic mechanism can be found by measuring the mean square displacement of clusters of different size. The second topic is the stability of clusters, i.e., their decay dynamics. The same microscopic mechanism governing diffusion also controls stability: if the diffusion is caused by evaporation and re-condensation, the cluster size is obviously unstable. It is expected to shrink if the cluster is surrounded by sinks for the evaporating atoms. The discussion of diffusivity and stability of large clusters is illustrated by recent experimental results, mainly obtained by scanning tunneling microscopy.

17:00

Lecture: P. Toennies, Max-Planck-Institut für Strömungsforschung, *Quasielastic helium atom scattering studies of microscopic surface diffusion: Experimental Results and Their Interpretation*

Quasielastic Helium Atom Scattering Studies of Microscopic Surface Diffusion: Experimental Results and Their Interpretation. P. TOENNIES, Max-Planck-Institut für Strömungsforschung. - - - Some case studies. Homogeneous metal systems, Na/Cu(001), CO on metal surfaces, summary and outlook.

17:50

Lecture: D. A. King, Cambridge University, *Reaction kinetics and spatiotemporal oscillations*

18:40

Lecture: U. Kuerpick, Kansas State University, *The role of vibrations in adatom diffusion*

The Role of Lattice Vibrations in Adatom Diffusion. U. KÜRPICK and T. S. Rahman, Department of Physics, Kansas State University, Manhattan, Kansas 66506, USA. - - - We investigate the role of lattice vibrations in self diffusion on Ag, Cu and Ni (100) surfaces within the framework of Transition State Theory. The vibrational entropy and vibrational free energy are evaluated from the local vibrational density of states. The latter is determined within the harmonic and quasiharmonic approximation. The potential energy surface and the force constant matrix are derived from the Embedded Atom Method. We find the contribution of the vibrational entropy to the diffusion coefficient to be significant. Furthermore the diffusion barriers are found to be temperature dependent.

Work supported by the Deutsche Forschungsgemeinschaft
and the U.S. National Science Foundation under grant No. DMR9120440

Thursday, August 29, 1996

9:00

Lecture: G. Comsa, IGV-KFA-Forschungszentrum,
Surface diffusion and film growth: I

Surface Diffusion and Film Growth: I. G. COMSA, IGV/KFA-Forschungszentrum Jülich, Germany. - - - A quick glance at the titles of the main Lectures of this NATO-ASI leads to an unexpected observation: although the overall subject is the atomistic and collective processes of surface diffusion, almost half of the titles include in a way or in another the word growth. This evidences how fashionable crystal growth nowadays is, but also that we can learn a lot about diffusion from the knowledge acquired recently in growth studies, simply because surface diffusion is the essential step in crystal growth. This is particularly true for the modern growth studies - mainly Molecular Beam Epitaxy (MBE) ones - which are performed far from equilibrium, and less for the classical near equilibrium processes. It might appear at first sight paradoxical that near equilibrium growth processes, in which practically all diffusion processes are active, are much less informative than far from equilibrium ones, where a more or less large part of these processes are frozen. By well conducted experiments, individual diffusion processes can be brought into play and thus the energetic hierarchy of these processes as well as each of them can be characterized.

In the first part, these general aspects of the relation between surface diffusion and growth will be discussed in more detail. In addition, the features and the applicability of some of the experimental methods - in particular thermal He-beam elastic scattering and scanning tunnel microscopy - used to characterize surface diffusion both directly as well as via the growth processes will be presented.

Surface Diffusion and Film Growth: II. G. COMSA, IGV/KFA-Forschungszentrum Jülich, Germany. - - - A quick glance at the titles of the main **Lectures** of this NATO-ASI leads to an unexpected observation: although the overall subject is the atomistic and collective processes of surface diffusion, almost half of the titles include in a way or in another the word growth. This evidences how fashionable crystal growth nowadays is, but also that we can learn a lot about diffusion from the knowledge acquired recently in growth studies, simply because surface diffusion is the essential step in crystal growth. This is particularly true for the modern growth studies - mainly Molecular Beam Epitaxy (MBE) ones - which are performed far from equilibrium, and less for the classical near equilibrium processes. It might appear at first sight paradoxical that near equilibrium growth processes, in which practically all diffusion processes are active, are much less informative than far from equilibrium ones, where a more or less large part of these processes are frozen. By well conducted experiments, individual diffusion processes can be brought into play and thus the energetic hierarchy of these processes as well as each of them can be characterized.

In the second part recent examples including studies of nucleation, of growth modes and of the surface growth morphology both near and far from equilibrium will be given and the resulting information on surface diffusion discussed.

11:10

Lecture: J. Evans, Ames Laboratory, *Submonolayer nucleation and growth, and transition to multilayer kinetic roughening during metal (100) homoepitaxy*

Submonolayer Nucleation and Growth, and Transition to Multilayer Kinetic Roughening During Metal (100) Homoepitaxy. J. EVANS, Ames Laboratory, Iowa State University, Ames, IA 50011 USA. - - - We describe realistic and comprehensive lattice-gas modeling of metal homoepitaxy. This work includes a detailed description of submonolayer nucleation and growth of two-dimensional islands as a necessary precursor to the description of multilayer kinetic roughening. Various features of the far-from-equilibrium film morphology are controlled by and provide information on rates or activation barriers for several key diffusion processes. At lower temperatures (T), submonolayer island densities reflect terrace diffusion barriers, and island shapes reflect diffusion barriers at island edges. The Arrhenius behavior of the island density for higher T reflects effective island dissociation rates. Island size distributions provide information on various of these parameters. Multilayer kinetic roughening is sensitive to the additional step-edge barrier for downward transport. We give examples of the precise determination of these barriers for several metal (100) homoepitaxial systems. We also discuss recent advances in the understanding of the shape of the island size distributions; transitions in "critical size"; the role of the downward funneling deposition dynamics in selecting the multilayer morphology; and the temperature dependence of kinetic roughening.

12:00

Lecture: Z. Zhang, Oak Ridge National Laboratory,
Dynamics of ad-dimers at surfaces

Dynamics of Ad-Dimers at Surfaces *Dynamics of Ad-Dimers at Surfaces.* Z. ZHANG, Solid State Division, Oak Ridge National Lab, P.O. Box 2008, Oak Ridge, TN 37831-6032. - - - Even a theorist agrees that a real surface contains a rich variety of defects, whose kinetic and thermodynamic properties are important issues in surface and materials science. In this talk, I will present results from recent theoretical and experimental studies of a few elemental types of point defects on Si(001), the substrate of choice for most microelectronic devices. Of particular note is a description of the recent controversies surrounding the energetics and dynamics of a Si ad-dimer on this surface. As a comparative study, the important roles of an ad-dimer as a block in influencing cluster mobilities and cluster stabilities on metal (100) surfaces will also be addressed.

17:00

Lecture: H. Metiu, University of California—Santa Barbara, *Beating the Time Scale in Computer Simulation of growth: From atom motion to coarsening*

Beating the Time Scale in Computer Simulation of growth: from atom motion to coarsening. Horia METIU, Department of Chemistry and Physics and QUEST, University of California, Santa Barbara, CA 93106, USA. - - - The diffusion of atoms controls island evolution during epitaxial deposition. To perform an atom-by-atom simulation of this process we must move tens of thousands of atoms for many seconds. The brute force “solution” solves Newton's equation for the adsorbed atoms and those of the substrate. This requires a time step of 10-15 seconds, the computer power needed to follow the system for a second is prohibitive. In this lecture I review the procedures used to avoid this time scale bottleneck. First we recognize that the site-to-site migration of an atom is an “isomerisation” reaction which is characterized by a probability that the jump takes place at a specified time. Since the reaction is first order this probability contains only one parameter, the rate constant. This can be calculated exactly (for a given potential energy) by using the correlation function theory. In the first section of the lecture I will show briefly how this is done. We can then define all the site-to-site jumps of importance to the aggregation process of interest and assign to each a rate constant. Once the rates are known we can design a kinetic Monte Carlo procedure which will execute each site-to-site jump with a frequency proportional to the rate of that jump. In section two we show how this procedure is implemented. Often these two steps put us in position of performing useful and realistic simulations. However, sometimes we have to perform simulations involving events that occur very rarely even within the kinetic Monte Carlo scheme. For example, the “evaporation” rate of an island atom to the surface of the substrate is substantially smaller than the rate of atomic diffusion around the edge of the island. If we want to simulate coarsening, evaporation is an essential event. However, to observe one evaporation event during the simulation we must execute billions of atomic movements around the border of the island. We cannot ignore these movements because they determine when an atom will evaporate. But following them makes the simulation impossible. This bottleneck is avoided by precomputing an evaporation probability as a function of the island size and temperature. Section three explains how this can be done and presents some results. Once the evaporation probability is known we can execute evaporation events, in a coarsening simulation, without having to move the atoms around the border of the island. The effects of this motion are already contained in the evaporation probability. This procedure cuts down enormously the computer time needed for studying coarsening. Finally, in the last section I we outline other applications of this strategy.

17:50

Lecture: G. Ehrlich, University of Illinois at Urbana—
Champaign, *Surface diffusion of metal atoms and clusters
directly observed*

Surface Diffusion of Metal Atoms and Clusters Directly Observed. G. EHRLICH, Materials Research Laboratory, University of Illinois at Urbana-Champaign, 1304 W. Springfield Ave., Urbana, IL 61801 USA. - - - Several techniques are now available for observing single atoms on surfaces, among them field ion microscopy, scanning transmission electron microscopy, as well as scanning tunneling microscopy. The information obtained by these methods during the past 30 years of studies on single metal atoms will be briefly surveyed, with special emphasis upon the atomic mechanisms of diffusion, as well as the qualitative description of diffusion on different metals. Recent quantitative studies of the diffusion of single atoms as well as of clusters will be presented which suggest that much still needs to be learned about diffusion processes.

Surfactant Mediated Hetero Epitaxy: Interplay of Diffusion, Strain Relief and Surface Morphology. M. HORN VON HOEGEN, Institute for Solid State Physics, University of Hannover, Germany. - - - Surfactants have been very effectively used for growth mode engineering of hetero epitaxial systems. For the growth of Ge on Si the monolayers of the elements Sb, As, Bi, and H have been tested to act as surfactant and force layer-by-layer growth of the Ge film. Without surfactant island formation is observed. The surfactant is not incorporated but segregates and floats on the growing Ge film. The driving force is the saturation of the dangling bonds of the semiconductor surface which strongly reduces the surface free energy and drives the strong segregation of the surfactant. The effect on the growth process is described by a selective change of activation energies for elementary diffusion processes.

Prior to the generation of strain relieving dislocations (below the critical thickness) the Ge film grows pseudomorphic with the Si lattice constant and is under strong compressive stress. The Ge film relieves strain by forming a rough and open surface on a nm-scale which allows for partial relaxation of the Ge towards its bulk lattice constant. At very high temperatures Ge on Si(100) forms cones with a uniform size of 30 nm covering the whole surface. The shape of the cones could be reversibly varied depending on the surfactant coverage and the elementary type of surfactant - i.e. by modifying the surface free energy.

After a particular critical thickness dislocations are finally generated. The microrough phase acts as nucleation centers for the dislocations. For Ge on Si(111) the dislocations form a quasi periodic array which is confined to the interface and exactly accommodates the lattice mismatch between Si and Ge. After deposition of only 4 nm of Ge a completely relaxed, defect free, and smooth Ge-film is observed. The use of atomic H as surfactant without doping and easy desorption will be discussed.

Friday, August 30, 1996

9:00

Lecture: M. Henzler, Universität Hannover, *LEED*
investigation of surface processes I

LEED Investigation of Surface Processes: I. M. HENZLER, Universität Hannover. - - - LEED (Low Energy Electron Diffraction) provides a variety of information on surfaces. Although diffusion is not measured directly, many processes, which include diffusion at some intermediate step, are well studied with LEED. Therefore, first a qualitative discussion will be given, what type of processes are of interest in this **Lecture**. The information needed for evaluation of the processes are essentially given in the spot profiles. Therefore, an overview over the evaluation of the spot profiles with respect to lateral and vertical distribution, to defects like steps, facets and point defects will be given. A well investigated non-equilibrium process is the epitaxial growth, especially under ultra high vacuum conditions, where LEED study is possible during growth. Especially the oscillation of the peak intensity has been used to determine the growth mode in homoepitaxy. Here the diffusion contributes to the nucleation and growth, so the barrier may be derived. A possible step edge barrier has a strong influence on the oscillation behavior. Examples for Pt on Pt(111) and Ag on Ag(111) will demonstrate the possibilities. In heteroepitaxy the misfit and the surface energies are additional parameters, which influence the growth. Other non-equilibrium processes, which include diffusion, are coarsening of islands (Ag on vicinal Ge). At finite temperatures surface arrangements may be in thermal equilibrium, nevertheless the diffusion provides a steady fluctuation of the arrangement. LEED studies are especially informative, which all surface atoms are involved in the fluctuations. Two examples will be studied: the roughening transition at the Cu(311) surface and the melting of a monolayer of Pb on top of Cu(111).

9:50

Lecture: P. Cohen, University of Minnesota, *Microscopic mechanisms of surface segregation: Sn doped GaAs (100)*

Microscopic Mechanisms of Surface Segregation: Sn Doped GaAs(100). P. I. COHEN, Department of Electrical Engineering, University of Minnesota, 200 Union St. SE, Minneapolis, MN 55455. - - - A submonolayer coverage of Sn, deposited before GaAs overgrowth, strongly modifies the growth processes on GaAs(100). This shows up most dramatically as strong beating in the RHEED intensity oscillations measured during growth. To understand the microscopic growth processes induced by the surface segregation of Sn, STM images of the evolution of GaAs(100) surfaces in a series of quenches of the growth front as well as in a series of annealing steps have been obtained. During growth, islands form due to the strain introduced by the Sn. After annealing in an As background, the islands attain a very narrow size distribution. When subsequently annealed in vacuum, these islands decrease in size, holes grow on the terraces, and on the lower side of step edges zones denuded of holes appear. The islands, terraces, and holes have a disordered (1×2) SnAs surface structure. The data is interpreted to show the existence of Sn in a bistable state in the GaAs surface. A qualitative model to explain the strong beats that are observed in measurements of RHEED intensity oscillations during growth is presented.

11:10

Lecture: A. Naumovets, Academy of Sciences of Ukraine,
*Surface diffusion and phase transitions in atomic
overlayers: I*

NAUMOVETS, Institute of Physics, NASU, 46 Prospect Nauki, Kiev-22, Ukraine.

- - - Overlayers on solid surfaces are remarkable for the diversity of lateral interactions between adsorbed particles which in particular is mirrored in the variety of surface phase diagrams. Lateral interactions affect surface diffusion (SD) even at the very low adsorbate coverages (below ~ 0.1 of a monolayer) through formation of adatom dimers and higher oligomers whose mobility is distinct from that of single adatoms. At high coverages in the initial deposit (e. g. above a monolayer) and under the condition of local quasiequilibrium the diffusion zone represents a display of all possible overlayer phases forming at the diffusion temperature and various coverages. Since different phases have different SD parameters, there occurs a self-organization of the diffusion zone: the phases with higher diffusivities occupy more extensive areas in the zone. Interesting points are the diversity of SD mechanisms in various phases and the possibility of the emergence of dissipative structures in SD.

The lecture will provide a review of investigations focused on correlations between SD and surface phase transitions.

12:00

Lecture: E. Conrad, Georgia Tech, *Entropic step doubling on (110) vicinal tungsten surfaces*
Entropic Step Doubling on (110) Vicinal Tungsten Surfaces.

E. CONRAD, School of Physics, Georgia Tech., Atlanta, GA 30332 USA. - - - While double atomic height steps have been observed on numerous vicinal surfaces, they always break up into two single height steps at higher temperature because of the increased mender entropy of two versus one step edge. We present LEED evidence from vicinal tungsten surfaces for the opposite situation, i.e. double height steps are preferred over singles at higher temperatures. The transition is driven because kinks on double steps are energetically favorable compared to kinks on single height steps. The nature of the transition will be discussed along with implications to self diffusion data on vicinal (110) tungsten surfaces.

Evening Session

Chairperson: Z. Zhang

17:00

Lecture: M. C. Tringides, Ames Laboratory & Iowa State University, *Adsorbate-adsorbate interactions and surface diffusion*

Adsorbate-adsorbate interaction effects in surface diffusion, M. C. TRINGIDES, Ames Laboratory, and Department of Physics and Astronomy, Iowa State University, Ames, IA 50011. - - -The analysis of surface diffusion becomes more complicated the presence of adsorbate-adsorbate interactions. The effect of the interactions results in coverage dependent diffusion coefficients. The activation energy measured in a given experiment has contributions from the adsorbate-substrate potential and the interactions. It is important to separate out each contribution. This can be done by comparing equilibrium experiments (which measure the relaxation of density fluctuations) with non-equilibrium experiments (which measure the ordering of domains). Such analysis will be illustrated with experiments on O/W(110) and Monte Carlo simulations on lattice gas models. Interactions also complicate the analysis of other experimental methods that measure surface diffusion. This will be illustrated with direct comparison between the fluctuation and concentration profile evolution methods on lattice gas models.

17:50

Lecture: M. Zinke-Allmang, University of Western Ontario, *Role of surface diffusion during late stage clustering*

Role of Surface Diffusion during Late Stage Clustering. M. ZINKE-ALLMANG, Department of Physics, University of Western Ontario, London, Ontario N6A 3K7, Canada. - - - Phase separation often occurs during thin film growth, as supersaturated surface layers are formed and evolve toward the thermodynamic equilibrium. These processes result in cluster formation and have to be taken into account in the interpretation of many surface science experiments since they compete with most phenomena, e.g., surface diffusion. In this talk two dynamic processes, dominant in the late stage of phase separation, will be studied in respect to their effect on surface diffusion.

(i) Ostwald ripening is the growth of large clusters at the expense of small ones under mass conservation, i.e., with no further deposition onto the surface. A mean field model will be introduced and we demonstrate that for most systems surface diffusion is the dominant mass transport process. This allows the determination of surface diffusion coefficients with high precision.

(ii) Coalescence describes the growth of all clusters after nucleation under an artificially raised supersaturation (e.g., deposition during molecular beam epitaxy) where cluster sizes increase mainly by merging upon contact. We will demonstrate that surface diffusion critically determines the early stages of clustering. Important conclusions on the dynamics of coalescence growth are drawn using surface diffusion to determine the age of a morphological feature.

The Interaction of a Ni and Si atoms with the Si (110) Surface. M. Menon^{a,b}, N. N. Lathiotakis^{c,d}, A. N. ANDRIOTIS^d, and J. E. Lowther^e ^a Department of Physics and Astronomy, University of Kentucky, Lexington, KY 40506-0055, ^b Center for Computational Sciences, University of Kentucky, Lexington, KY 40506-0045, ^c Physics Department, University of Crete, P.O. Box 1470, Heraklio, Crete, Greece 71409, ^d Institute of Electronic Structure and Laser, Foundation for Research and Technology-Hellas, P.O. Box 1527, Heraklio, Crete, Greece 71110, ^e Department of Physics, University of Witwatersrand, Johannesburg, South Africa. - - - The reconstruction of Si(110) surface and chemisorption of Ni and Si atoms on this surface are investigated using the tight-binding molecular dynamics (TBMD) scheme incorporating Green's function methods that allows an efficient embedding of a subspace in a semi-infinite substrate. Our chemisorption studies reveal a striking contrast between Si and Ni atoms in their behavior with respect to bonding on the surface. Additionally, in their most stable chemisorbed configuration, Si and Ni are found to induce changes in the surface reconstruction that is qualitatively distinct.

Lecture: M. Asscher, Hebrew University, *Optical studies of surface diffusion: SHG diffraction experiments and simulations*

Optical Studies of Surface Diffusion: SHG Diffraction Experiments and Simulations. M. ASSCHER, Zhao Wei, and R. W. Verhoef, Department of Physical Chemistry and the Farkas Center for Light Induced Processes, The Hebrew University, Jerusalem 91904. - - - Simulations of monolayer grating formation using laser induced thermal desorption (LITD) suggest that very interesting information on lateral interactions among neighbor adsorbates can be obtained from Fourier transform analysis of the coverage profiles formed. The Fourier components directly correlate with the experimentally measurable diffracted second harmonic generation (SHG) from these gratings. It has been found that the intensity of the second and higher order diffraction signals oscillate in a unique way as a function of desorption laser power and initial coverage. This behavior of the higher order diffraction peaks is predicted for cases of strong lateral repulsion or attraction between neighbors and it is not seen for non interacting adsorbates.

The same analysis is employed to study diffusion of adsorbates on surfaces. The decay in time of the diffraction signals provides direct information on surface diffusion. It was found that as a function of diffusion time, the intensity of higher order diffraction peaks oscillate for cases of repulsion and attraction among neighbor adsorbates while gradual decay is always observed in the case of no interaction. The first order diffraction peak, on the other hand, decays for all cases of lateral interactions and for all initial coverages and laser powers, therefore cannot be used to obtain information on lateral interactions. The behavior of higher order diffractions can thus be utilized to learn on the type and magnitude of interactions between adsorbates on surfaces as they affect both desorption and surface diffusion. The predictions are experimentally checked for the system of K on Re(001).

Finally, we demonstrate how useful the comparison of experimental results with MC simulations of surface diffusion can be for a particular case of strong repulsion among neighbors - NH_3 on Re(001).

Monday, September 2, 1996

9:00

Lecture: R. J. Behm, Abteilung Oberflächenchemie und Katalyse, *Nucleation and growth in epitaxy—beyond simple, site independent hopping diffusion, I*

Mass Transfer in Surface Chemical Processes: Adsorption, Faceting, and Reaction on Ag(110). J. E. REUTT-ROBEY, Department of Chemistry and Biochemistry, University of Maryland, College Park, MD 20742 USA. - - - Virtually all surface chemical processes involve mass transfer. Relating mass transfer in surface chemical systems to atomistic events presents a challenging experimental and theoretical problem. I will describe scanning tunneling microscopy experiments that track mass flow during adsorption, faceting, and reaction on Ag(110). At room temperature on the clean surface steps fluctuate freely. A Langevin analysis indicates that the step motions are dominated by detachment/attachment kinetics with an exchange interval of *ca.* 350 ms per step site. Upon exposure to oxygen, silver adatoms participate in the formation of a ...Ag-O-Ag... added-row reconstruction. The ability of the step edge to supply adatoms and "keep up" with the rate of oxygen arrival is tested. Above a critical oxygen pressure of $\sim 10^{-5}$ mbar, the rate of oxygen atom arrival exceeds the thermal detachment rate of silver adatoms from the step edge. Nonetheless, ordered oxygen overlayers continue to form, obtaining the necessary silver adatoms by the creation of large vacancy nuclei and by accelerating step motion. Thus, even for the simple process of chemical adsorption, several distinct mass-transfer mechanisms are accessible. I then discuss mass transfer processes in two surface chemical reactions involving O/Ag(110). In the CO₂-formation reaction, carbon monoxide reacts with surface oxygen, releasing silver adatoms from the added rows. The silver adatoms return to the step edge, on a timescale that reflects rapid terrace diffusion and edge-attachment kinetics. In the CO₃-formation reaction, in contrast, the silver adatoms released by reaction do not return to the steps, but are retained locally in reconstructions that support the carbonate adlayer. Finally, in related studies on vicinal Ag(110) surfaces, oxygen adsorption leads to more global mass flow, breaking the surface up into large O-covered (110) facets and O-free step bunches. These faceting dynamics are investigated as a function of step density and orientation. Examples of faceting via nucleation and via spinodal decomposition are presented and the underlying mass transfer is related to microscopic surface properties.

11:10

Lecture: T. Tsong, Academia Sinica, *Diffusion of single atoms and small atom clusters on terraces and stepped surfaces: II*

Diffusion of Single Atoms and Small Atom Clusters on Terraces and Stepped Surfaces: II. T. T. TSONG, Institute of Physics, Academia Sinica, Taipei, Taiwan 11529 ROC. - - - Using field ion microscope and scanning tunneling microscope, it is possible to study the diffusion behavior of single atoms and small atomic clusters on flat terraces and stepped surfaces of metals and semiconductors. I will discuss the basic principles and methods of these studies emphasizing our recent studies on stepped surfaces. Diffusion behavior of single atoms and small atom clusters at lattice steps has a great effect on the surface structure of epitaxial films.

12:00

Lecture: P. Ruggerone, Fritz Haber Institut, *Microscopic processes behind homoepitaxial growth of metallic systems I*

Microscopic Processes behind Homoepitaxial Growth of Metallic Systems.

P. RUGGERONE*, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin. - - - A microscopic and complete theory of epitaxial growth in all its stages is still not available. Within the framework of a Monte Carlo scheme we have studied the homoepitaxial growth of Al on Al(111) and of Ag on Ag(100). The simulations use microscopic energetic parameters that are the results of accurate Density Functional Theory calculations. The importance of prefactors in determining the island shape during the growth is particularly stressed for the (111) surface. For Ag on Ag(100) the layer-by-layer growth that is observed experimentally for a wide temperature range as well as the compact shape of the islands is discussed.

* Work done in collaboration with A. Kley, B. D. You, and M. Scheffler.

17:00

Lecture: M. Scheffler, Fritz-Haber-Institut der Max-Planck-Gesellschaft, *Theory of surface diffusion and crystal growth*

Self-ordering of Nano-structures on GaAs Surfaces I. M. SCHEFFLER, Fritz-Haber-Institut der Max-Planck-Gesellschaft. - - - Formation of quantum dots and quantum wires with properties satisfying device requirements on those structure's size, shape, uniformity, and density became possible by utilizing self-ordering phenomena on crystal surfaces. In this talk I will discuss two basic theoretical aspects which crucially influence the growth of nano-scale structures: 1) self-diffusion of cations on AlGaAs surfaces, and 2) an analysis of surface energies and stress relief. While the first is relevant for the formation of quantum wires on V-grooved substrates, the latter determines the shape of quantum dots.

Work done in collaboration with E. Pehlke, A. Kley, and N. Moll

17:50

Lecture: C. Teichert, Max-Planck-Institut für
Mikrostruktur-physik, *Stress-driven morphological changes
of SiGe Films grown on vicinal Si(001) substrates*

Stress-Driven Morphological Changes of SiGe Films Grown on Vicinal Si(001) Substrates. C. TEICHERT, Max-Planck-Institut f. Mikrostruktur-Physik, Halle/Saale D-06120, GERMANY. - - - During the growth of SiGe films on vicinal Si(001) the resulting growth front undergoes a series of strain relief mechanisms. Two of these are: ripple formation due to bunching of the preexisting substrate steps, and the formation of {105} faceted three-dimensional (3D) islands. Ex-situ atomic-force microscopy was used to study quantitatively the evolution of these morphological features in a SiGe/Si superlattice as a function of substrate miscut. It was found that, while the 3D islands usually exhibit a broad size distribution for a single alloy layer, they are organized into an array of uniformly sized crystallites upon growing a superlattice. In general, these crystallites are four-sided pyramids. For specific substrate miscuts an interplay of ripple formation and facetting yields a regular array of prism-like "hut-clusters". The stress-driven step-bunching and the self-organization of the 3D islands are explained in the framework of continuum elasticity theory, and the underlying mechanisms are discussed in terms of surface diffusion processes.

Tuesday, September 3, 1996

9:00

Lecture: R. Gomer, University of Chicago, *Recent results
from the fluctuation method: II*

The equilibrium shape and the "vapor" pressure of an island. Horia METIU, Department of Chemistry and Physics and QUEST, University of California, Santa Barbara, CA 93106, USA. - - - Thermodynamic concepts such as the equilibrium shape of an island, its vapor pressure and the "surface tension" of its edge, have been used to study the islands formed during epitaxial deposition. In spite of its success the use of thermodynamics in this context leads to some difficulties. Prior to the discovery of STM thermodynamics has been applied to systems containing at least 1012 molecules. But, since an island is a large molecule, STM performs routinely "one molecule measurements". Therefore we have to examine how we should apply thermodynamics to one molecule system. Furthermore, as far as thermodynamics is concerned, STM measurements are rather imperfect: they have nothing to say about either heat or work. They can only measure island sizes and shapes, and their fluctuations. Given these limitations, how much can we learn by using thermodynamics? The starting point in our analysis is the observation that thermodynamics deals with average quantities, defined over an appropriate Gibbs ensemble. In the first section we introduce a Gibbs ensemble that uses kinetic Monte Carlo simulations to define the equilibrium shape and study its fluctuations. In the second section we examine the concept of "surface" tension (a better name would be edge tension) in this ensemble and its connection to the equilibrium shape. This leads to a simple extension of the Wulf construction to the case of two-dimensional islands. The third section is concerned with the "vapor pressure" of an island and its use to define the island's surface tension. We also examine island size fluctuations and discuss their thermodynamic implications. In section four we use the detailed balance and thermodynamics to propose a formula for the size dependence of the evaporation rate. It is well known from statistical mechanics that all ensembles (i.e. canonical, grand canonical, etc.) lead to the same physical results if the system is sufficiently large. If the system is small, or if one intends to study fluctuations, this equivalence between various ensembles is no longer true. The consequences of this are examined in section five. Throughout the lecture we calculated the work on the bulk of the island by ignoring its crystallinity; and we have also ignored the effect of electrostatic interactions between the atoms forming the island, which could be important for the III-V or II-VI semiconductors which have "ionic" surfaces. In the last section of the lecture we discuss how the inclusion of these two effects might change the thermodynamic equations. All thermodynamic concepts discussed in the lecture are defined and "measured" through kinetic Monte Carlo simulations; thus thermodynamics is obtained from hopping rates (i.e., diffusion constants) only. The concepts developed here can, in principle, be applied to real STM measurements. Unfortunately, getting good statistics is more tedious in laboratory than in simulations.

11:10

Lecture: M. Henzler, Universität Hannover, *LEED*
investigation of surface processes II

12:00

Lecture: S. Stoyanov, Bulgarian Academy of Sciences,
*Diffusion and electromigration of Si adatoms on vicinal Si
surfaces—formation and relaxation of bunches of steps*

Diffusion and Electromigration of Si Adatoms on Vicinal Si Surfaces - Formation and Relaxation of Bunches of Steps. S. S. STOYANOV, Bulgarian Academy of Sciences, Institute of Physical Chemistry, Sofia, 1113, Bulgaria. - - - The hypothesis for electromigration of Si adatoms on Si surfaces has been explored in an attempt to reproduce the bunching of steps, observed in many experiments on sublimation by heating the crystal with a direct current through it. Equations of step motion have been derived in the framework of two different models: 1) BCF model, assuming that the steps are boundaries, effectively separating the transport processes (and the concentration fields) at neighboring terraces; 2) A model describing the case of low rate of atom detachment from the steps and high mobility of the adatoms (in this limit the dominating process at the crystal surface is the surface transport due to electro- migration, whereas the steps are weak sources of adatoms). Analytical treatment of the simplest case - a bunch of 2 steps results a simple formula, relating the steady state interstep distance with the electromigration force and the step-step repulsion force. Numerical integration of the equations of step motion has been used in an attempt to reproduce the experimentally observed time evolution of the vicinal Si surface under direct current heating. This approach provides some ground to estimate the effective charge of the Si adatoms as well as the step- step repulsion force.

Wednesday, September 4, 1996

9:00

Lecture: J. Villain, Centre d'Etudes Nucléaires de Grenoble, *Epitaxial clusters: Equilibrium properties vs. kinetics*

Kinetic coefficients in a system far from equilibrium. Paolo Politi and J. VILLAIN, Centre d'Etudes Nucléaires de Grenoble. - - - The kinetic coefficients in a growing surface are very different from their equilibrium value. Assuming deposition of particles from a beam on a initially flat surface of high symmetry orientation and neglecting evaporation, the kinetic coefficient relevant at the beginning of the growth is evaluated in 1+1 and 2+1 dimensions. It is the sum of three terms: i) a term coming from an "equilibrium" chemical potential, which vanishes with temperature but diverges at low flux in the case of a singular surface; ii) a term, whose origin is the random character of nucleation, which depends only on the beam intensity and the diffusion constant but is independent of the temperature and of the atomic distance; iii) a term deriving from the fluctuations of the diffusion current, which depends upon the beam intensity, the diffusion constant and the atomic distance. In 1+1 dimensions, it is independent of the temperature. The validity of a linear equation is limited to small slopes $|m| < 1/\ell_c$, where ℓ_c is the maximum terrace width.

Effects of Surfactants on Surface Diffusion. D. KANDEL, Weizmann Institute of Science, Department of Physics of Complex Systems, Rehovot 76100, Israel. - - - In various experiments on surfactant mediated semiconductor epitaxy, a high surface density of two dimensional islands has been observed. This result has been interpreted as an indication that surface diffusion is suppressed. Here we propose an alternative model where surfactants enhance surface diffusion, and also passivate island edges. The two models lead to different dependences of island density N on flux F in the submonolayer regime, and can therefore be distinguished experimentally. A rate equations approach suggests that if surface diffusion is suppressed, N is proportional to $F^{2i/(i+2)}$, where i is the critical island size. On the other hand, if our model applies, N is proportional to $F^{2i/(i+3)}$. The latter functional dependence is consistent with recent experiments on silicon homoepitaxy using chemical vapor deposition.

11:10

Lecture: R. J. Behm, Abteilung Oberflächenchemie und
Katalyse, *Nucleation and growth in epitaxy—beyond simple,
site independent hopping diffusion: II*

12:00

Lecture: P. Feibelman, Sandia National Laboratory, *A chemical view of bonding and diffusion at surfaces: II*

A Chemical View of Bonding and Diffusion at Metal Surfaces: II. P. J. FEIBELMAN, Sandia National Laboratory, Albuquerque, NM 87185-1413. - - -
Despite the delocalized nature of electrons in metals, elementary chemical ideas, including coordination, valence-saturation and directional bonding, are indispensable guides to the systematics of adatom-metal potential energy surfaces. Drawing from first principles total energy calculations, as well as atomic resolution microscopy data, I will illustrate the application of "chemical thinking" in the (often predictive!) analysis of representative examples. I will discuss the promotion-hybridization view of surface structure and bonding, and show its relevance to materials stability in recent work on "liquid metal embrittlement." I will review the "chemistry" of cluster diffusion and concerted substitution, and explore the systematics of adatom binding near surface defects.

Work supported by the U.S. Department of Energy under contract DE-AC04-94AL85000.

17:00

Lecture: S.-C. Ying, Brown University, *Study of surface diffusion through Langevin dynamics*

Study of Surface Diffusion Through Langevin Dynamics Outline of Two Lectures:

II. S. C. YING, Department of Physics, Brown University, Providence, Rhode Island 02912. - - - We present in these two lectures the theoretical investigation of adatom diffusion based on Langevin dynamics. In the first lecture, we derive a Generalized Langevin Equation from a microscopic Hamiltonian and discuss its application to the study of surface diffusion. In particular, we focus on how the diffusion constant depends on the friction parameter characterizing the non-adiabatic coupling of the adatom to the substrate excitations. We will discuss such topics as the validity of the transition state theory, occurrences of long jumps and memory effects in determining the prefactor and the barrier for surface diffusion. In the second lecture, we discuss the application of the formalism to two specific systems. The first system is adsorption on W(100) which undergoes a displacive phase transition. We show that the friction and hence the diffusion constant exhibits anomalous temperature dependence near the transition due to critical fluctuations. The second system is Na/Cu(001) for which there are extensive data from recent Helium Atom scattering experiments. We will demonstrate that through a careful analysis of the extensive set of data, the entire potential energy surface of the adsorption system (PES) as well as the friction can be determined. This yields a complete information for the adatom dynamics beyond the simple determination of the diffusion constant.

17:50

Lecture: I. Markov, Bulgarian Academy of Sciences,
*Surface energetics form nucleation data analysis in
homoepitaxy*

Surface Energetics from Nucleation Data Analysis in Homoepitaxy. I. V. MARKOV, Institute of Physical Chemistry, Bulgarian Academy of Sciences, Sofia 1113, Bulgaria. - - - Analysis of experimental data on nucleation on surfaces is far from the state of a routine procedure. This is illustrated on the example of 2D nucleation on Cu(001) (Zuo et al., *Phys. Rev. Lett.* **72**, 3064 (1994); Duerr et al., *Surf. Sci.* **328**, L517 (1995)). The reinterpretation of the data leads to the result that the observed change of the slope of the Arrhenius plot of the island separation can be explained by a change of the mechanism of diffusion from concerted substitutional mechanism at low temperatures with an energy barrier of 0.24 eV to bridge-hopping mechanism at higher temperatures with an energy barrier of 0.45 eV, rather than by a change of the number of atoms in the critical nucleus from 1 to 3.

18:15

Lecture: X. Xiao, Hong Kong University of Science & Technology, *Impurity effects on surface diffusion: S, O, K on CO/Ni(110)*

Impurity Effects on Surface Diffusion: S, O, K on CO/Ni(110). X. XIAO, Department of Physics, Hong Kong University of Science and Technology, Yuanlin Xie, Christian Jakobsen, and Y. R. Shen, Department of Physics, University of California, Materials Sciences Division, Lawrence Berkeley Laboratory, Berkeley, CA 94720. - - - A small amount of coadsorbed species could significantly alter the surface diffusion of CO on Ni(110). The three elements reported here are sulfur, oxygen, and potassium with the former two as "poison" and the latter as "promoter" in catalytic hydrogenation reactions. All three are found to impede CO diffusion by drastically changing the apparent activation energy and preexponential factor. The apparent diffusion activation energy E_D increases from clean surface value of 2-3 kcal/mol to a saturation of ~8 kcal/mol as the amount of impurities increases, with minor differences in the saturation value for the three elements. The strength of the impeding effect decreases from S to O to K. Detail mechanisms for the effects will be discussed for all three elements, with the first two being identified as blocking diffusion through impurities modified steps and the latter one as affecting diffusion by strong interaction with CO on terraces.

Thursday, September 5, 1996

9:00

Lecture: A. Naumovets, Academy of Sciences of Ukraine,
*Surface diffusion and phase transitions in atomic
overlayers: II*

Surface Diffusion and Phase Transitions in Atomic Overlayers: II. A. G. NAUMOVETS, Institute of Physics, NASU, 46 Prospect Nauki, Kiev-22, Ukraine.

- - - Overlayers on solid surfaces are remarkable for the diversity of lateral interactions between adsorbed particles which in particular is mirrored in the variety of surface phase diagrams. Lateral interactions affect surface diffusion (SD) even at the very low adsorbate coverages (below ~ 0.1 of a monolayer) through formation of adatom dimers and higher oligomers whose mobility is distinct from that of single adatoms. At high coverages in the initial deposit (e. g. above a monolayer) and under the condition of local quasiequilibrium the diffusion zone represents a display of all possible overlayer phases forming at the diffusion temperature and various coverages. Since different phases have different SD parameters, there occurs a self-organization of the diffusion zone: the phases with higher diffusivities occupy more extensive areas in the zone. Interesting points are the diversity of SD mechanisms in various phases and the possibility of the emergence of dissipative structures in SD.

The lecture will provide a review of investigations focused on correlations between SD and surface phase transitions.

9:50

Lecture: X. Zhu, University of California—Davis, *Recent results of hydrogen diffusion on Ni(111) at low temperatures: Searching for the evidence of quantum tunneling diffusion of hydrogen on Ni(111)*

Recent Results of Surface Diffusion of Hydrogen and Deuterium on Ni(111) from 150 K to 65 K. X. ZHU, Department of Physics, University of California, Davis, CA 95616 USA. - - - Using the method of optical diffractions from laser-induced adsorbate density gratings and varying the grating spacing from 16microns to 0.38 microns, we have extended the measurement of the diffusion of hydrogen and deuterium on Ni(111) from 150 K to 65 K. The diffusion coefficients of hydrogen and deuterium on Ni(111) at an averaged coverage below 0.2 changes by as much as 5 orders of magnitude over this temperature range. For hydrogen, it appears that an activated diffusion with an energy barrier of 2.5 kcal/mol continues from 150 K to 65 K. For deuterium, an activated diffusion with an energy barrier 3.6 kcal/mol continues from 140 K to 90 K (over 3 orders of magnitude in diffusion coefficient). We did not observe signs of quantum tunneling diffusion even with the diffusion coefficient being as small as 2×10^{-15} cm²/sec. We will discuss the significance of these new results in terms of our present understanding of light atom diffusion on and in metals at low temperatures.

11:10 Lecture: C. Uebing, Physikalische Chemie,
*Monte Carlo simulation of surface diffusion on
homogeneous and heterogenous surfaces*

Monte Carlo Simulation of Surface Diffusion on Homogeneous and Heterogeneous Surfaces. C. UEBING, Physikalische Chemie, Postfach 140 444, Duesseldorf D-40074, Germany. - - - Experimental investigations of surface diffusion on such surfaces are a challenge for state of the art surface science. Recently some new techniques for measuring surface diffusion coefficients of adsorbates on macroscopic surfaces have been developed¹ and it is obviously of interest to increase our general understanding of surface diffusion.

In recent years lattice gas models have been introduced to study the effects of adsorbate-adsorbate interactions and surface heterogeneity on surface diffusion. In many cases even lattice gas models are too complicated for exact analytical treatments of the diffusion problem especially if ad-ad interactions are taken into consideration, and only in some exceptional cases general equations for the description of surface diffusion can be derived.^{2,3} However, the Monte Carlo method constitutes a powerful tool to analyze surface diffusion, and it has been shown in previous publications that this method is extremely valuable to improve our understanding of adatom diffusion on homogeneous and heterogeneous surfaces.^{4,6}

¹ R. Gomer, *Rep. Prog. Phys.* **53**, p. 917 (1990).

² V. P. Zhdanov, *Surf. Sci. Lett.* **149**, p. L13 (1985).

³ D. A. Reed and G. Ehrlich, *Surf. Sci.* **102**, p. 588 (1981).

⁴ C. Uebing and R. Gomer, *J. Chem. Phys.* **95**, p. 7626 (1991).

⁵ C. Uebing and R. Gomer, *Surf. Sci.* **306**, p. 419 (1994).

⁶ C. Uebing, *Phys. Rev. B* **49**, p. 13913 (1994).

12:00

Lecture: J. Wollschlaedger, University of Hannover,
*Epitaxial growth of Mg/Ag(100): Transition from complete
condensation to adsorption-desorption equilibrium*

Epitaxial Growth of Mg on Pd(100) and Ag(100). J. WOLLSCHLAEDGER,
Institut für Festkörperphysik, Appelstr. 2, D-30161 Hannover, Germany. - - - The
epitaxial growth of Mg adlayers deposited on Pd(100) and Ag(100) has been studied by
SPA-LEED. In the submonolayer range Mg grows with $c(2 \times 2)$ structure on both
substrates. The intensity oscillations of the (00) beam demonstrate that Mg starts to grow
pseudomorphically in the layer-by-layer growth mode. At room temperature 3D islands are
formed on top of these pseudomorphic layer. For Ag the non-vanishing intensity of both
the specular beam and the $(1/2 \ 1/2)$ spot recorded simultaneously during deposition
observed at high temperature can be explained by an equilibrium between adsorbing and
desorbing Mg atoms. Thus under these conditions no 3D islands are formed.

17:00

Lecture: Gomez-Rodriguez, Universidad Autonoma de Madrid, *Scanning tunneling microscopy study of single Pb atom diffusion on Si(111) 7×7 and Si(111) 5×5 surfaces*

Scanning Tunneling Microscopy Study of Single Pb Atom Diffusion on Si(111) 7×7 and Si(111) 5×5 Surfaces. J. M. GOMEZ-RODRIGUEZ^a, J.-Y. Veuillen^b, A. M. Baro^a, and R. C. Cinti^b, ^a Departamento de Fisica de la Materia Condensada, Universidad Autonoma de Madrid, 28049-Madrid, Spain. ^b Laboratoire d'Etudes des Proprietes Electroniques des Solides, CNRS, 38042-Grenoble Cedex 9, France. - - - The very early stages of Pb deposition on Si(111) 7×7 and Si(111) 5×5 surfaces have been investigated in real time by scanning tunneling microscopy (STM). The STM results show that single Pb atoms are highly mobile at room temperature inside (7×7) or (5×5) half-cells but diffuse at very low rates to neighbor half-cells. Variable temperature measurements combined with unusually long periods of imaging time¹ have enabled us to measure the activation energy for the diffusion of single atoms between different half-cells on the Pb/Si(111) 7×7 system.

¹ J. M. Gomez-Rodriguez, J.J. Saenz, A.M. Baro, J.-Y. Veuillen and R.C. Cinti, *Phys. Rev. Lett.* **76**, 799 (1996).

17:25

Lecture: G. Vidali, Syracuse University, *Investigations of adsorption, recombination and desorption of H on low temperature surfaces of bare and ice-covered silicates*

Investigations of Adsorption, Recombination, and Desorption of H on Low Temperature Surfaces of Bare and Ice-Covered Silicates. G VIDALI, Department of Physics, Syracuse University, 201 Physics Building, Syracuse NY 13244-1130. - - -We report experimental investigations of HD production following adsorption of H and D at thermal energies on a silicate surface (olivine) in the 5-15 K range. Flash desorption experiments have been conducted to yield desorption energies, order of desorption and recombination coefficients over a wide range of coverage. Significant recombination occurs only at the lowest temperatures. Current models of diffusion and recombination of H on inert and cold surfaces developed to explain interstellar recombination processes will be discussed and appraised in the light of the new results.

17:50

Lecture: M. Jalochoowski, Institute of Physics UMCS,
*Low-temperature epitaxial growth of thin metal films: in
situ electrical resistivity study*

Low-Temperature Epitaxial Growth of Thin Metal Films: In Situ Electrical Resistivity Study. M. JALOCHOWSKI, Institute of Physics, Maria Curie-Skowska University, Pl. M. Curie-Skodowskiej 1, PL-20031 Lublin, Poland, M. Hoffmann, and E. Bauer, Physikalisches Institut, Technische Universitaet Clausthal, D-38678 Clausthal-Zellerfeld, Federal Republic of Germany. - - - We have studied the growth of ultrathin Pb films on Si(111) surfaces at very low temperatures by resistivity measurements. The structure of the layers was monitored by reflection high-energy electron diffraction (RHEED). Clear evidence of correlation between growth mode and the electrical resistivity variations was found. The quantum-size-effect (QSE) theory was used for a quantitative analysis of the data. The presence of the surface roughness and volume impurities and their impact on the resistivity was taken into account. In order to modify the interaction of growing Pb with the substrate the Si(111) surfaces with (7×7) , $(\sqrt{3} \times \sqrt{3})$ -Pb, $(\sqrt{3} \times \sqrt{3})$ -Ag and (6×6) -Au reconstructions were produced. Both the growth mode and the electrical resistivity were strongly influenced by the substrate morphology. Co-deposition of Pb with small amount of Ag at low temperatures enhanced the QSE effects in the resistivity and prolonged the layer-by-layer growth. Further increase of the Ag amount destroyed the epitaxial growth at about 15 at.% of Ag. Co-deposition of Pb with In enabled to reach layered growth within whole range of the Pb/In ratio. Steady layer-by-layer growth over thickness range exceeding hundred of the monoatomic layers was observed at about 40 at.% of In. The role of the domain size during low-temperature epitaxial growth is discussed.

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Friday, September 6, 1996

9:00

Lecture: M. Altman, Hong Kong University of Science and Technology, *Impact of step edge barriers in step flow growth studied by LEEM*

LEEM Investigations of Step Flow Growth: Impact of Step Edge Barriers. M. ALTMAN, Department of Physics, Clear Water Bay, Kowloon, Hong Kong. - - - Step flow is one of the basic mechanisms of crystal growth. According to the seminal work of Burton, Cabrera and Frank (BCF), the steady state, non-equilibrium adatom concentration on a terrace during step flow growth is related to the even solution of a wave-like equation governing the supersaturation.¹ This solution is a symmetric function of position with respect to its peak at the middle of a terrace. The peak value increases as a function of terrace width until nucleation is driven on terraces wider than some critical terrace width. The step flow velocity, which is related to the gradient of the adatom concentration at the step position, increases nearly linearly as a function of terrace width for small terrace widths.

Using low energy electron microscopy, we have measured the critical terrace width for step flow as a function of temperature for Si/Si(111) (7×7) growth. An Arrhenius behavior is seen with activation energy of 2.05 eV. The distribution of island nucleation positions on a terrace at the critical terrace width has also been measured. This distribution is a probe of the adatom concentration during growth. A small shift of the concentration peak towards the up-step side of a terrace has been observed. This shift is accounted for analytically by including the previously neglected odd solution to the BCF supersaturation wave equation. An asymmetric concentration profile may result from a step edge barrier (barrier to descend a step minus the surface diffusion barrier) to diffusion. For Si(111), our results indicate a negative step edge barrier. The dependence of step flow velocity upon terrace width was found to be in qualitative agreement with the BCF results. Step flow on surfaces with strong asymmetry [Si(100)] and with known positive step-edge barrier [Ag(111)] will also be discussed.

¹ W. K. Burton, N. Cabrera, and F. C. Frank, *Phil. Trans. Roy. Soc. London A* **243** 299 (1951).

Diffusion Coefficient for Interacting Lattice Gases - Random Potential Approach. M. A. ZALUSKA-KOTUR^a, Lukasz A. Turski^b, and Zbigniew W. Gortel^c, ^aInstitute of Physics, Polish Academy of Sciences, and College of Science, Al. Lotników 32/46, 02-668 Warszawa, Poland. ^bCenter for Theoretical Physics, Polish Academy of Sciences and College of Science, Al. Lotników 32/46, 02-668 Warszawa, Poland. ^cDepartment of Physics and Theoretical Physics Institute, University of Alberta, Edmonton, T6G 2J1 Edmonton, Alberta, Canada. - - - Diffusion in interacting adsorbate is analyzed with use of master equation for the lattice gas model. Chemical diffusion coefficient for a diluted, interacting adsorbate is calculated using concepts of diffusion theory in a disordered medium in which the random potential is related to the local field felt by each particle due to interparticle interactions. We use the random local field method to evaluate distribution of local fields in the equilibrium state. Results for the simplest lattice gas with attractive interactions are successfully compared with Monte Carlo simulations. Diffusion in adsorbate undergoing order-disorder phase transformation is analyzed for the lattice gas model with repulsive interactions. The role of thermodynamic factor is discussed. A more complex system of particles interacting with nearest and next nearest neighbors is studied using a projection onto the simple Potts model. Results for systems with long range interactions of dipolar type are presented.

Atomic Mobility of Ag and Fe on the Ag(100) Surface. M. H. LANGEAAR and D. O. Boerma, Nuclear Solid State Physics, Materials Science Centre, Nijenborgh 4, Groningen University, The Netherlands. - - - In order to understand the (epitaxial) growth of the Fe/Ag(100) multilayer system it is important to gain insight in various atomic processes like mobility of adatoms and clusters, and diffusion mechanisms. In this work Low Energy Ion Scattering is used to look at the mobility of Ag and Fe adatoms and clusters on a Ag(100) surface. The surface was irradiated with a 3.0 to 6.0 keV Ne+ or Ar+ beam and the yield of scattered (and recoiled) particles was measured. Large sensitivity for adatoms and clusters on the surface is obtained by measuring in a geometry with glancing incoming or exit angle. By using TOF (Time-Of-Flight), mass separation of the scattered and recoiled particles is obtained. We measured the thermal stability of the adatoms and clusters and determined the activation barrier for Ag adatom mobility on the Ag(100) surface. Furthermore we determined the temperature at which the exchange mechanism for Fe adatoms on the Ag(100) surface becomes important. In order to fully understand the measured spectra a LEIS simulation program was developed. In this program incoming trajectories are linked with reversed-time outgoing trajectories of scattering and/or recoiling events at the surface. In this procedure the trajectories as well as the energies are matched.

*Studies of Surface Diffusion Under Non-Equilibrium Conditions.*I. VATTULAINEN, Research Institute for Theoretical PhysicsP.O. Box 9, University of Helsinki, FIN-00014, Finland. - - - STUDIES OF SURFACE DIFFUSION UNDER NON-EQUILIBRIUM CONDITIONS

I. Vattulainen(a,b), J. Merikoski(a,b,c), T. Ala-Nissila(a,b,d),
and S. C. Ying(b)

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Surface diffusion plays an important role in many surface phenomena such as epitaxial growth, catalysis, and ordering. In addition to its practical significance, surface diffusion is a challenging research topic also from the theoretical point of view. Some of the most intriguing questions at present concern the non-equilibrium properties of surface diffusion, since many non-equilibrium phenomena such as surface growth are very important for applied science, but a rigorous theoretical understanding is lacking. In this work, we consider surface diffusion under nonequilibrium conditions, after a quench from a totally random initial state to a temperature characterizing an ordered state. The ordering dynamics is studied by extensive Monte Carlo simulations using a lattice-gas model for the O/W(110) system. We first introduce the concept of { ν mobility} which characterizes the motion of the adatom under non-equilibrium situations. The time-dependence of the tracer and collective mobilities thus defined are calculated within several time slices, which are determined according to the decay of the excess energy. The mobilities are then fitted to an Arrhenius form to extract the effective diffusion barriers that are shown to be strongly time-dependent during the ordering process. For comparison, the equilibrium properties have also been determined. We discuss our results in light of available experimental data, and consider the difficulties associated with interpreting non-equilibrium measurements.

11:10

Lecture: T. Linderoth, University of Aarhus, *Real-time imaging of the diffusion, nucleation, and growth of Pt on Pt(110)*/K. Morgenstern, University of Aarhus, *Adatom and vacancy island decay at variable temperatures*

Real-Time Imaging of the Diffusion, Nucleation and Growth of Pt on Pt(110). T. R. LINDEROTH, S. Horch, L. Pedersen, E. Laegsgaard and F. Besenbacher, Institute of Physics and Astronomy, University of Aarhus. - - - Using variable-temperature STM, Pt adatoms on the Pt(110)-(1×2) surface are studied in the sub-monolayer coverage regime. We find the adatom hopping rate to be of the order of minutes at room temperature. This system therefore provides a fascinating new opportunity to follow diffusion, nucleation and growth in real time at the atomic level. The adatoms are confined to the troughs of the missing-row reconstruction, causing the diffusion to be one-dimensional. In the temperature range from 10 C (where diffusion sets in) to 50 C, the migration of single adatoms, as well as their nucleation and the growth and stability of the resulting 1D islands is monitored using STM-movies. Dimer break-up is frequently observed, whereas larger islands are predominantly stable. From the temperature dependence of the adatom migration, a diffusion barrier is extracted. The issue of tip-influence on the diffusivity is addressed. For deposition temperatures from 80 C to 130 C, conventional "quench-and-look" growth experiments are performed, and the resulting island size distributions are analyzed. Above 100 C, nucleation frequently occurs on top of the islands, even at very low coverage, indicating that upwards diffusion has become feasible. Kinetic Monte-Carlo simulations are used to determine a barrier for this and other key processes.

Adatom and Vacancy Island Decay at Variable Temperatures.

K. MORGENSTERN, G. Rosenfeld, E. Laegsgaard, F. Besenbacher, Institute of Physics and Astronomy, University of Aarhus, Ny Munkegade, Aarhus C 8000, Denmark. - - -

The decay of monatomic islands on Ag(111) has been studied in the temperature range from 250 K to 350 K. The continuum theory that – based on the Ostwald ripening theory – allows to describe the decay analytically includes assumption about the surroundings of the decaying islands that usually differ considerably from the experimental facts. The use of this theory is then limited to a qualitative understanding of the decay behavior. A major theoretical assumption is a circular border surrounding the decaying island at a large distance. This border acts as a sink or a source for the adatoms that detach from the adatom island or fill the vacancy island, respectively. We designed the surface, so that this hypothetical border is present in the shape of an ascending step edge encircling the decaying island. This defined geometry allows the understanding of the differences in decay behavior between the two island species in a more than a qualitative way.

Diffusion of Large Clusters: Experiments and Simulations. P. JENSEN, University Lyon-1, CNRS, 69622 Villeurbanne Cedex, FRANCE. - - - We study the formation of thin films prepared by cluster deposition both experimentally and theoretically. From the experimental side, we have studied deposition of carbon, antimony, gold clusters on several substrates. Our results are reviewed in P. Melinon et al., "From free clusters to cluster assembled materials," *Int. J. of Mod. Phys. B* **9**, 339-397 (1995)). To understand the first stages of the film growth, and, specifically, the *diffusion* of the clusters, we have developed a model which takes into account the three basic ingredients of the growth: Deposition, Diffusion, and Aggregation of the clusters. Details are given in P. Jensen et al., *Nature* **368**, 22 (1994) and *Phys. Rev. B* **50**, 15316 (1994). We have applied the model to the deposition of antimony and gold clusters containing 250 and 2300 atoms. A comparison of the experimental results and the model predictions has allowed the measure of the *diffusion* constant of the clusters on the surface (for preliminary results, see L. Bardotti, P. Jensen, *Phys. Rev. Lett.* **74**, 4694 (1995)). We will present our new results on gold cluster diffusion and the microscopic diffusion mechanisms suggested by our molecular dynamics simulations.

Transport Coefficients in a Transient State on a One-Dimensional Lattice. R. KUTNER¹, P. Pendzig², D. Knödler², and R. Przenioslo^{1,1}, ¹ Department of Physics, Warsaw University, PL-00681 Warsaw, Hoza 69, Poland, ² Fakultät, Universität Konstanz, D-78434 Konstanz, Germany, - - - The work consists of two parts. In the first part we extend the linear response analysis to calculate the complex dynamic mobility/conductivity for a system in a transient state relaxing to equilibrium. This analysis has a meaning in the intermediate time and frequency region for example, for solvation dynamics and nonlinear relaxation in electrolyte systems. The discussed situation differs from the one considered by the usual linear response theory since our system during its relaxation is still under the action of an external force. It relaxes and simultaneously somehow responds to the applied force. As a test model we assumed a single-particle one-dimensional random walk on a lattice in an inhomogeneous (random) periodic potential where a transient state is created by a nonequilibrium initial probability distribution. Using spectral analysis we derived spectral and summed formulas for the above mentioned dynamic quantities. The feature which distinguishes the present result is a force-dependence, since summed formulas depend, in general, on the external force but do not depend on its amplitude. A time- and frequency-dependent diffusion coefficient was also studied. As a striking effect, we found a non-monotonic frequency and time dependence of transport coefficients. The dc values are well described by the usual linear response expressions for thermalized system. The relation between the dynamic mobility and the frequency-dependent diffusion coefficient is still an open question for the system in a transient state. In the second part the systematic numerical simulation were performed by exact enumeration and by Monte Carlo method. By this way a one-dimensional random walk of a single ion in a Coulombic potential well has been studied as an example.

Theory of Coherent Island Growth. H. DOBBS, Interdisciplinary Research Center for Semiconductor Materials, Imperial College, London SW7 2BZ, England.

- - - The possibilities of growing ensembles of nearly identical quantum boxes has attracted attention to the nucleation and growth of coherent three-dimensional (3D) islands during heteroepitaxy. We study this process using a self-consistent rate equation analysis. The effect of misfit strain is to cause the two-dimensional (2D) islands which form during submonolayer deposition to reconfigure themselves as 3D islands with increasing probability as they grow larger. However, because of the rapid detachment of atoms with strain-weakened bonds from 2D islands, only a small fraction grow sufficiently large to make this transition to a 3D configuration. As growth proceeds, most of the deposited material is taken up by the 3D islands that do form. Although these allow a much greater strain relaxation, there is a concentration of the strain field at the island edges that inhibits the attachment of adatoms. In cases where the height to width (aspect) ratio of the 3D islands increases during growth, the attachment barrier limits the eventual size of the islands, and also can give rise to a comparatively narrow distribution of island sizes. Our results show that although 3D island growth during heteroepitaxy is a general phenomenon, only a narrow window of deposition flux and temperature will generate a system which could be usefully exploited as quantum boxes.

Work performed in collaboration with Andy Zangwill and Dimitri Vvedensky
Interdisciplinary Research Centre for Semiconductor Materials, Imperial College, London SW7 2BZ, United Kingdom.

Poster Abstracts

P-01

Anomalous diffusion in non-equilibrium systems. E. ARAPAKI^a, P. Argyrakakis^a, M. C. Tringides^b, ^aSolid State Section, Physics Department, Aristotle U. of Thessaloniki, Greece, ^bAmes Laboratory* and Department of Physics and Astronomy, Iowa State University, Ames, IA USA. - - - We study tracer diffusion in the 2-dimensional Ising model with attractive interaction J under non-equilibrium conditions. The jumping probability depends only on the initial site energy. We calculate $\langle R^2 \rangle$ the mean square displacement averaged over all the particles for different J/kT ratios where T is the temperature. The system shows sublinear dependence on time for ratios below the transition temperature into the ordered (1×1) phase and for early enough times. This can be related to the evolution of the ordered domains. For sufficiently long times linear dependence is observed which signifies that equilibrium is attained. We determine the transition times $t_c(T)$ where this crossover to the linear dependence occurs. In addition, we calculate the waiting time distribution for different temperatures. At low enough temperatures it shows a power law decay with time with the exponent related to the exponent describing the sublinear dependence of $\langle R^2 \rangle$ in the same temperature regime.

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P-02

Heterogeneous Precipitation of Silicon Oxide Using Laser-Induced Centers. Yu. BLUMS, A. Medvid', Riga Technical University, General Physics, la Kalklu str., Riga, LV-1658, Latvia. - - - In this work, the possibility to use laser-induced centers as nuclei for the precipitation of oxygen in silicon wafers is under investigation.

After the generation of additional centers in silicon during the laser annealing by Q-switched Nd:YAG laser, Si wafers were subjected to two-step thermal treatment in helium atmosphere (50 h at 550 C and 10 h at 1050 C) for initiation of the oxygen precipitation. After the selective etching of laser annealed and thermally treated samples was detected, that a size of etching features on surface with the laser induced centers increased (up to 5-10 mkm), but their concentration decreased ($35-50 \text{ cm}^{-2}$), in comparison with size and concentration of the etching features on surface without the laser induced centers (accordingly 2-5 mkm and $120-140 \text{ cm}^{-2}$). Such an unhomogeneous distribution of etching defects exists in 24-28 mkm thick layer of wafer.

This unhomogeneous distribution of the etching features is related with oxygen precipitation process. The dependence of this effect on the oxygen content in silicon crystal, concentration of laser induced centers, duration of thermal treatment is under investigation.

P-03

Relation Between Chemical Surface Diffusion Coefficient and Order of the Layer. P.-L. CAO, Physics Department, Zhejiang University, Hangzhou 310027, People's Republic of China. - - - Using lattice gas model and time dependent Monte Carlo method, we calculated the chemical surface diffusion coefficients with nearest neighbor and next nearest neighbor interactions directly from Fick's law. Our results show that the chemical diffusion coefficient depends on the structure of the adsorbate layer. In the case of repulsive nearest neighbor interactions when $\epsilon_{nn}/KT \geq 2.0$, ordered lattice gas phase $c(2 \times 2)$ is established near $c=0.50$. For repulsive next nearest neighbor interactions, as $\epsilon_{nnn}/KT \geq 2.0$, $p(1 \times 2)$ and $p(2 \times 1)$ structures are coexisting near $c=0.50$. These ordered domains will greatly reduce the chemical surface diffusion coefficient.

P-04

Diffusion of Single Adatoms in Two Periodic Coupled Dimensions. G. CARATTI, R. Ferrando, R. Spadacini, G. E. Tommei, Dipartimento di Fisica dell'Università di Genova, CFSBT/CNR and INFN, via Dodecaneso 33, 16146 Genova, Italy. - - - The Brownian motion of single atoms adsorbed on a solid surface is investigated on the basis of the Fokker-Planck Equation (FPE) in the surface position and velocity variables. The interaction between an adatom and the substrate is modeled by a square 2D coupled "egg-carton" potential and a friction force. The extension of the Matrix Continued Fraction Method to two dimensions leads to the solution of the FPE and consequently a complete study of the diffusion coefficient in all relevant potential barriers and friction regimes is performed. A comparison of the exact results with the widely employed 1D diffusion path approximation indicates that dimensional effects are always present and more relevant at low friction. A "quasi-2D" analytical approximation is derived and discussed in the overdamped regime. The hopping rate and long jump probabilities for activated diffusion are evaluated. It turns out that the x - y coupling has the effect of lowering the diffusion coefficient, the jump rate and multiple jumps probabilities with respect to the decoupled case. This is particularly evident in the underdamped regime, the most important for surface diffusion.

Metastable Growth of 2D Pb on Ge(001). D. CVETKO, Laboratorio TASC-INFM, Padriciano 99, 34012, Trieste, Italy. - - - Hetero-epitaxial growth of Pb on the Ge(001) surface has been studied in -situ by high resolution He atom scattering (HAS). For low substrate temperatures (140 K) an apparent 2D growth with Pb layer wetting the Ge substrate occurs, whereas for higher substrate temperatures Pb grows by 3D islands (Stranski-Krastanov mode). Moreover, upon heating to room temperature the layer-by-layer grown Pb film irreversibly transforms to 3D islands. We have examined carefully the low temperature growth. Initially, several highly corrugated Pb overlayer structures, commensurate with the underlying Ge(001) surface are formed, whereas later on, the film structure switches to the Pb(111) symmetry with extremely low diffracted-to-specular ratio, characteristic of close-packed metal surfaces. Further Pb deposition results in strong specular oscillations. These specular oscillations though perfectly reproducible, for a finite number of layers display a highly irregular pattern in time. A similar behavior has been observed for Pb/Cu(111)¹ and Pb/Cu(100),² and attributed to an interplay between a single and double layer growth caused by a quantum size effect (QSE) of the growing Pb film.³ In the case of Pb/Ge(001) a careful examination of the specular peak profile $I(\text{DK}, \text{Dkz}, \text{coverage})$ reveals that the upper-most monatomic step height of the growing Pb(111) film varies strongly with the number of deposited layers, which makes the usual relation between the diffracted intensity in a fixed-scattering-condition-experiment and the surface morphology poorly defined. Initially, the lead step height values have been found to oscillate between $d_i = 2.5 \text{ E}$ and $d_i = 3.1 \text{ E}$, but with the increasing film width (after a few tens of layers) they gradually damp-out, to reach the Pb(111) bulk interatomic distance $d = 2.86 \text{ E}$. The question whether all interlayer spacings of the film or just the outermost one is affected at present remains open.

¹Hinch B. J., Koziol C., Toennies J. P., and Zhang G., *Europhys. Lett.* **10**, 341 (1989).

²Zeng H. and Vidali G., *Phys. Rev. Lett.* **74**, 582 (1995).

³Feibelman P. J., *Phys. Rev. B* **27**, 1991 (1983).

Study of the Diffusion of Lennard-Jones Clusters. P. DELTOUR, Department de Physique des Materiaux, Universite Claude Bernard Lyon-1, 69622 Villeurbanne Cedex, France. - - - Recent work carried out in our group has allowed us to measure the diffusion constant of large clusters on surfaces.

We want to understand the microscopic mechanisms behind cluster diffusion. For this, we study the diffusion of Lennard-Jones clusters of different sizes on a surface using molecular dynamics. We have measured the dependence of the cluster diffusion on the substrate temperature and lattice parameter.

We will also present results obtained in two extreme cases :

- (1) the cluster is moving freely on a frozen lattice and
- (2) the cluster is moving as a solid body on a thermalized lattice.

We finally present interpretations of these simulations in terms of possible diffusion mechanisms.

P-07

Vibrational Modes and Relative Stability of Stepped Surfaces of Cu. S. DURUKANOGLU, Department of Physics, 116 Cardwell Hall, Kansas State University. - - - We present a systematic study of the vibrational thermodynamic properties of the vicinals of the (100) and (111) surfaces of Cu, in the harmonic approximation of lattice dynamics. The local vibrational density of states are evaluated using a real space method with the force-constant matrix generated from semi-empirical potentials based on the embedded atom method. The relative stability of the (331), (211) and (511) surfaces, chosen because of similar step-step separation and because they are prototypes of 3 different types of step geometry, is examined through consideration of the Helmholtz free energy. We find that steps on Cu(211) and Cu(511) are more stable than their counterparts on Cu(331). We discuss these results in the light of the differences in the surface geometry. Additionally, polarizations of the step localized modes on all three surfaces are traced back to the changes in the atomic surface force constants. Frequencies of the surface modes and their dispersion are compared with available experimental data.

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P-08

In Situ Study of Kinetic Roughening During Homoepitaxial Growth. P. F. Miceli and W. C. ELLIOTT, University of Missouri, Columbia, MO 65211, T. Tse and P. W. Stephens, SUNY - Stony Brook. - - - Kinetic roughening during film growth involves many diffusive mechanisms. Atomic mobility across terraces, over step-edges and along island edges all contribute to the evolving surface morphology during growth. In order to address these issues, we have used x-ray scattering to study the temperature and orientation dependence of Ag homoepitaxy. Because the barrier to diffusion over a step-ledge is much larger for the (111) orientation than for the (001), qualitatively different growth is observed for these surfaces and this allows us to quantify the effects of a large barrier on the evolving surface roughness.

We find the rms roughness of the Ag(111) surface grows as a power-law in time with exponent $\beta=1/2$ for temperatures between 150 K and 300 K, undergoing a transition to lower values at higher temperatures. This behavior is due to the additional step-ledge barrier to diffusion being insurmountable in the low temperature regime. The Ag(001) surface also displays power-law growth, but with smaller values of β . This is interpreted as the (001) surface having a smaller step-ledge barrier relative to the barrier to diffusion on a terrace.

Activated Transition of Chemisorbed Hydrogen into Subsurface Sites on Pd(311). D. FARÍAS, M. Patting, and K. H. Rieder, Fachb. Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany. - - - The interaction of hydrogen with a Pd(311) surface was studied by means of He diffraction and thermal desorption spectroscopy. At 120 K, the formation of (2×1)H, (2×1)2H, (2×1)3H and c(1×1)H phases was observed, with coverages 0.25 ML, 0.50 ML, 0.75 ML and 1 ML, respectively. The TDS data show three desorption states: α at ~ 170 K, β_1 at ~ 285 K and β_2 at ~ 310 K. In all four hydrogen phases, the chemisorbed H-atoms desorb in the β_2 state, whereas the β_1 state is originated by H-atoms located at subsurface sites. From a quantitative analysis of the He-diffraction data, we found that in the three (2×1) phases the H-atoms are adsorbed near to the threefold hollows on the (111) facets. In all four phases, long-range order disappears at ~ 180 K. These order-disorder transitions were found to be completely reversible for the (2×1)H and (2×1)2H phases upon heating to 220 K and subsequent cooling to 120 K. For the (2×1)3H phase, however, a very different behavior was observed: heating to 220 K leads to the migration of 0.25 ML H-atoms into subsurface sites, and the (2×1)2H phase is recovered after cooling down to 120 K. This effect is observed *only if* the coverage of the disordered layer is > 0.5 ML, indicating that it is not only controlled by the surface temperature but also by the equilibrium properties of the disordered overlayer, i.e. surface diffusion processes. All these results suggest that the mechanism involved in the population of subsurface sites on Pd(311) is very different to the one present on Pd(110), where it is driven by a pairing-row reconstruction of the substrate.^{1,2} On Pd(311), on the contrary, no evidence for a substrate reconstruction has been found in any of the three (2×1) phases.

¹R. J. Behm, V. Penka, M. G. Cattania, K. Christmann and G. Ertl, *J. Chem. Phys.* **78** (1983) 7486.

²K. H. Rieder, M. Baumberger and W. Stocker, *Phys. Rev. Lett.* **51** (1983) 1799.

P-10

Anisotropy of Surface Diffusion Determined by Study of Ordering Kinetics: Oxygen on (011) Molybdenum. A. G. FEDORUS and V. F. KOVAL, Institute of Physics, National Academy of Sciences of Ukraine Prospekt Nauki 46, Kyiv-22, UA-252022, Ukraine. - - - Kinetics of ordering in one-fifth-monolayer oxygen film adsorbed on Mo(011) is studied to derive data on surface diffusion. Evolution of the $c(2 \times 2)$ domain average size occurring after upquench of the overlayer preliminarily deposited at low temperature is investigated by video LEED. The two-dimensional diffraction intensity profile is monitored in a wide range of times at different ordering temperatures and corresponding average domain sizes are calculated. Time dependence of the domain size fits the power law $\langle L \rangle = At^x + B$ with the growth exponent $x = 1/2$ and the rate constant A dependent on ordering temperature. The growth exponent proves to be of the same value in any direction. However the domain growth rate is found to be different along the $\langle 001 \rangle$ and $\langle 011 \rangle$ axes. The diffusion coefficient D is considered to relate to A as $D^x \sim A$. The diffusion anisotropy can be thus determined: $D_{001}/D_{011}=2$. This ratio turns out constant, independent of temperature, showing the equality of the activation energy $E_d=1.76$ eV for the two directions. The results are discussed in comparison with the data on E_d and model calculations of diffusion anisotropy obtained for the considered system in other works.

P-11

Correlated Jump-Exchange Processes in the Diffusion of Ag on Ag(110). R. FERRANDO, Dipartimento di Fisica, Università di Genova, Italy. - - - The high-temperature diffusion of silver adatoms on Ag(110) is studied by molecular dynamics simulations. Silver is modeled by many-body potential derived in the framework of the second-moment approximation to the tight-binding model. Single and long jumps along the $[1\bar{1}0]$ direction and cross-channel exchanges are found at the lowest temperature considered in the simulations (450 K); simple exchanges are possible along the $[001]$ direction and in the diagonal direction, essentially with the same probability. Correlated events involving both jumps and exchanges become important as the temperature is raised to 600 K.¹ These events can be of the jump-exchange, exchange-jump, exchange-exchange kinds, or even more complicated and, above 600 K, they amount to about one quarter of the total exchanges. The appearance of these events is related to the strong anharmonic vibrations of the row atoms in the top surface layer.

¹R. Ferrando, to appear in *Phys. Rev. Lett.* 76, 4195 (1996).

Atomic Force Microscope Investigation on LPCVD Polysilicon Surface During Thermal Annealing. C. FLUERARU, K. van der Werf*, N. van Hulst*, and D. Dascu, Institute of Microtechnology, P. O. Box 38-160, Bucharest 72225, Romania, * Department of Applied Physics, University of Twente, P.O. Box 217, 7500 AE Enschede, The Netherlands. - - - Polycrystalline silicon (polysilicon) is playing an important role in microelectronics device such as bipolar integrated circuits, MOC device, solar cells and thin film transistors. In characterizing polysilicon films the Atomic Force Microscope (AFM) have been used because of its nanometer resolution in real space.¹ The most important parameters of polysilicon which can influence significantly the device properties are surface roughness and grain size.

The polysilicon film was grown, on thermally oxidized silicon, by low pressure chemical vapor deposition (LPCVD) at 570° C and 620° C temperatures. The surface topography of polysilicon was visualized using AFM. As was expected² the surface roughness of a deposited indoped polysilicon is lower at 570° C than at 620° C deposition temperature.

Then the sample was thermal annealing at 600° C during 168 h and in order to see the changes in surface morphology at each 6 h the surface topography was analyzed with AFM.

The paper is focus on surface morphology measurements of polysilicon induced by thermal annealing.

The z-mode without feedback gives cantitative information on surface topography, the error signal made provides a high contrast image of the surface. The torsion parameter monitors the movement of the cantilever perpendicular to the deflection direction. This parameter gives information friction forces between tip and surface. An evaluation of friction coefficient versus surface morphology is presented. The comparison of the friction force images obtained for different scan directions can help distinguish between topographical and tribological contrast. There are several forces responsible for a deflection of the cantilever: adhesive forces which originate from a water layer between tip and sample, electrostatic forces, van der Waals forces, magnetic forces, ionic forces and other.³ The adhesive water layer force is by far the largest 10^{-8} - 10^{-7} N.

It should be noted that the RMS roughness values do not give a full description of the surface. The fractal dimension may be calculated with relative ease from AFM image. The RMS roughness gives the "amplitude" of the surface roughness, while the fractal dimension can be interpreted as the "frequency" of the roughness.⁴

¹K. O. van der Werf et al., *Rev. Scientific Instrum.* **64**, 10,2892 (1993).

²E. Ybok, S. Garb, *J. Electrochim. Soc.* **140**, 2927 (1993).

³C. Flueraru, D. Dascalu, *Rom. J. of Physics* (in press).

⁴S. Chester et al., *Solid State Tech.* (Jan. 1991).

P-13 *Trapping Effects in Surface Diffusion.* L.K. GALLOS and P. Argyrakis, Solid State Section, Physics Department, Aristotle U. of Thessaloniki, 54006 Thessaloniki, Greece. - - - We consider the problem of random walkers diffusing on a lattice surface, containing a random distribution of static traps in a small given concentration. The particles could be some kind of excitation or a chemical species, while the trapping centres could correspond to sites where the excitation is dissipated, or another chemical species which upon reacting causes the disappearance of the other species. We present analytical solutions and numerical results for trapping processes on such a surface. The survival probability of random walkers is studied and it is found that it is related to the distribution of the number of distinct sites visited on the lattice.

P-14 *Elevated-Temperature STM Study of Ge and Si Growth on Si(001) from GeH₄ and Si₂H₆.* I. GOLDFARB, J. H. G. Owen, K. Miki, and G. A. D. Briggs, University of Oxford, Department of Materials, Parks Road, Oxford OX1 3PH, England. - - - We have used high-temperature UHV STM to monitor the MBE growth of Si and Ge from gas sources on Si(001) surface. The purpose of this study was to get a better understanding of growth kinetics, with a view to future studies of the growth of alloys and superlattices. In many cases, gas-source MBE has been proven to yield better results than solid-source MBE. We wish to identify the reaction pathway from the initial GeH₄ and Si₂H₆ in the gas phase up to the final stage of Ge and Si layers growing on the substrate. Therefore, special attention was paid to the initial stages of epitaxy, at submonolayer coverages. We have observed similarities and differences in the growth behavior of Ge and Si. In particular, hydrogen plays a crucial role below 600 K, by blocking the available substrate sites. In the case of Ge growth, various phenomena were observed, such as surface roughening, missing dimer trenches and segregation to specific surface sites, such as SB-type step edges and missing dimer defects.

P-15

Effect of Strong Entropic Repulsion of Surface Diffusion of Polymer Chains.

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² Department of Physics, Box 1843, Brown University, Providence, RI 02912, USA.

- - - We have studied the diffusion of flexible chains on surfaces using the fluctuating bond model¹ and Monte Carlo simulations. We have computed various time dependent correlation functions in order to extract both tracer and collective diffusion coefficients of the chains as a function of density. To calculate collective diffusion coefficients for various chain lengths we have also used the Boltzmann-Matano method. Unlike tracer diffusion, collective diffusion coefficient shows unusual behavior as a function of concentration. It first increases, but after reaching a maximum value goes to zero as the coverage approaches unity. We have developed an analytical theory, which shows that this kind of behavior is due to strong entropic repulsion that increases with increasing length and flexibility of the chains. The theory agrees well with simulation results.

¹I. Carmesin and K. Kremer, *J. Phys. France.* **51** (1990) 915.

P-16

Evolution of Surface Morphology: A Variable-Temperature STM Study.

M. S. HOOGEMAN, M. F. Chang, M. A. J. Klik, J. W. M. Frenken, FOM-Institute for Atomic, and Molecular Physics, Kruislaan 407, 1098 SJ Amsterdam, The Netherlands. - - - We present a variable-temperature STM-study of the annealing of

out-of-equilibrium structures on Ni(001). The out-of-equilibrium structures are produced by sputtering. Thanks to the extremely low thermal drift in our microscope¹ we monitor the entire anneal process in real time over several hundreds of degrees, without interrupting the experiment for mechanical adjustment of the tip or surface position.

We find that, depending on the precise amount of removed material, the surface morphology evolves towards equilibrium along two entirely different pathways: Ostwald ripening or growth by coalescence. This reflects itself in differences in the large-scale patterns that form and the time and temperature dependences of the restoration processes. We explain these differences in terms of the atomic-scale diffusion mechanisms responsible for the surface mass transport.

¹M. S. Hoogeman, D. Glastra van Loon, R. W. M. Loos, J. J. van der Linden, L. Kuipers, M. F. Chang, M. A. J. Klik, B. K. Ambrose, T. J. Palmer, and J. W. M. Frenken, to be published.

Surface Morphologies in Sputter Deposition and Ion Beam Assisted Deposition of Pt on Pt(111). M. KALFF, Institut fuer Grenzflaechenforschung und Vakuumphysik, Forschungszentrum Juelich, GmbH, D 52425 Juelich, GERMANY.

- - - Formation of 2D islands and the island density in homoepitaxially grown films on a Pt(111) surface are determined by adatom diffusion. Ion beam assisted deposition (IBAD) and sputter deposition (SD) are often used in technical applications. The aim of these studies is to understand the nucleation mechanism in those deposition techniques. The morphologies are examined by a variable temperature scanning tunneling microscope (STM) in a UHV chamber.

At first IBAD-experiments are used to investigate the influence of a defined quantity of ions with controlled energy on the morphology. Ar-ions with energies of 400 eV and 4000 eV during vapor deposition of Pt lead to a dramatic increase of the island density. It is demonstrated that the increase in island density is due to adatom clusters formed by the bombardment with ions.

In the second group of experiments sputter beam deposited Pt films are examined. Here similar results are observed, although no ion beam is directed onto the sample. This can be explained by the fact, that a fraction of the reflected ions and sputtered Pt-atoms reach the sample surface with high energies. These secondary energetic atoms have similar effects on the morphology as an ion beam directed onto the sample. The contribution of the secondary energetic atoms is investigated by changing the deposition geometry which results in a variation of the amount of these atoms. Additional experiments show that the coverage of films deposited at 300 K is reduced after an annealing of the sample to 710 K. During this annealing process bulk and surface vacancies created by energetic bombardment recombine with adatoms.

To describe these effects quantitatively the amount of reflected and sputtered atoms is calculated. The effect of the deposited atom energy on the morphology is simulated in a computer program. The results of this simulation fit well the result of the experiments.

Further experiments with a coverage of 5 ML show that films grown by IBAD and sputter deposition grow smoother than those deposited by PVD, i.e., less uncovered atomic layers in the STM images. Some arguments for this behavior are discussed.

P-18 *Activation Free Energy for Selfdiffusion Processes on Metallic Surfaces.* G. KOPIDAKIS, Physics Department, Technical University of Denmark, Lyngby DK-2800, Denmark. - - - We study the adatom selfdiffusion on various metallic surfaces. A Monte Carlo method is used to find the free energy differences between the adatom located in the stable hollow site and in the transition state within the effective medium theory. The resulting hopping rates are then compared for several systems.

P-19 *Reaction Diffusion Systems of Type $A + B \rightarrow 0$.* Z. KOZA, University of Wroclaw, Institute of Theoretical Physics, Pl. Maxa Born 9, PL-50204 Wroclaw, Poland. - - - We review recent developments in the field of the reaction-diffusion systems of the type $A + B \rightarrow 0$, including experiments, theory and simulations. A special attention is paid to anomalous and universal properties of such systems.

P-20 *The Experimental Optical Research of the Dynamics Surface's Variation at High Temperature Conditions in Vacuum.* A. S. KOZLOVA, Moscow Aviation Institute, Moscow, Russia. - - - Under the effect of high temperature and vacuum the properties of metals considerably change, therefore, to know strength, elasticity, wearability, and corrosion resistance characteristics at normal low temperature is not enough in designing space structures.

The most informative methods are the optical ones. For the first time a research group of P. I. Lebedev Physical Institute AS USSR¹ experimentally obtained the reflection factor dependence for massive metals on riveting stick presence disappearing in the process of its annealing.

On the basis of Taylor's photometric sphere² original techniques have been developed to obtain metal reflection factor temperature dependence in vacuum for optical and close IR wave range.

The study of reflection factor temperature histories of metal samples in vacuum showed that in the process of its heating the reflection factor of a polished surface increases approximately by 30 - 40%. The analysis of niobium and molybdenum temperature histories allows to establish a reflection ability dependence of their surface on the process of oxide appearance, their modification change and their fuming. Thus, it is possible by applying metal and alloy reflection factor temperature history to determine the most favorable, i.e., optimum operating mode of metal structures in deep vacuum.

¹Golovashkin A. I. et. al., Optical Properties of Niobium II, *Journ. ET Ph*, **56** (1), 51, 1969.

²Taylor A. H., The Measurement of Diffuse Reflection factors and New Absolute Reflectometer, *J. Opt. Soc. of Amer.*, **4**, 1920.

Quantum Diffusion Calculations of H on Ni(001) Using a Model Potential Based on First Principles Calculations. T. R. MATTSSON, Lennart Bengtsson, Göran Wahnström, Department of Applied Physics, Chalmers University of Technology and Göteborg, University, S-412 96 Göteborg, Sweden, Bjork Hammer CAMP, Department of Physics, Building 307, Technical University of Denmark, DK-2, 800 Lyngby, Denmark. - - - Hydrogen diffusion on metal surfaces has been a subject of great interest both theoretically and experimentally due to the pronounced quantum behavior at low temperatures.

Common to most theoretical approaches are the use of different model potentials where the parameters are chosen to fit a set of data. So far limited experimental data, mainly from the hollow site, have been the only reliable source of information but a correct treatment of tunneling processes needs data in the barrier region. We have performed first principles calculations of the total energy using DFT together with the GGA II approximation for the exchange-correlation functional and constructed a model potential by fitting to the first principles data. The model potential reproduces both the first principles and experimental data in a good way.

Using the path-centroid formulation we calculate the transition rate and we find a marked change of the temperature dependence for the diffusion constant around 60 K, indicating that quantum tunneling starts to dominate the diffusion process.

K. MEINEL, H. Wolter, Ch. Ammer, I. Sebastian, K. Wandelt, H. Neddermeyer, Martin-Luther-Universitdt, Halle-Wittenberg, Fachbereich Physik, Halle D-06099, Germany. - - - The surface diffusion of epitaxial Cu films on Ru(0001) is drastically modified by adsorbed oxygen. Using STM this phenomenon has been demonstrated by investigating growth and stability of Cu/Ru(0001) thin film systems at temperatures between 300 and 500 K. During the film growth oxygen floats on top of the Cu film and acts as a surfactant. It strongly reduces the diffusion length of the deposited Cu atoms and causes a large density of two-dimensional nuclei. This effect forces a perfect layer-by-layer growth at temperatures around 400 K where pure Cu films show a Stranski-Krastanov growth behavior. The stability of ultrathin Cu films (thickness < 3 monolayers), however, is drastically reduced by oxygen. Adsorbing oxygen abruptly causes a layer-by-layer removal of the Cu films accompanied by the formation of three-dimensional islands even at temperatures around 500 K. The film decomposition is analyzed by considering characteristic strain structures indicating the thickness of the films.

TiO₂ Crystal Growth on Titanium Metallic Surface Heated at High Temperatures. M. MOMIRLAN, Institute of Physical Chemistry, Romanian Academy, Splaiul Independentei 202, Bucharest 77208, Romania. - - - The studies of the oxidation of titanium were carried out at high temperatures.

Titanium samples were kept in an electric vertical furnace for one hour in ambient air, at 900°, 1000°, and 1100°. The weight of the titanium plates was measured after the oxidation process. After cooling, the layer of titanium oxide formed on the surface of the metallic samples was examined by electronic microscopy.

The oxide crystallites were photographed enlarged 200, 500, 1000, 3000, and 30000 times. The form and size of the microstructure were examined.

At 900° C a film of nearly cubic crystals of 0.7-7 µm was obtained. Pin shaped crystals of 3 to 10 µm were also observed.

When the oxidation temperature was 1000°C a layer of lamellar and acicular crystals of 1,6 to 20 µm was noted.

At 1100° C long lamellar particles of 8 to 34 µm were formed. Some hexagonal crystals of 2-3 µm were also observed.

The diagrams suggested that the increase of crystals is dependent of temperature reaction.

B. MUELLER, Institut de Physique Experimentale (IPE), DP-EPFL, PHB-Ecublens, CH-1015 Lausanne, Switzerland. - - - Island shapes can be varied or even tailored by choice of external parameters in molecular beam epitaxy. In an extended substrate temperature and flux range, noncompact islands with dendritic or fractal shape have frequently been found on triangular or hexagonal but not on square lattices. The difference in shape is explained by the higher barrier of edge diffusion on triangular lattices due to the presence of two-fold coordinated edge sites. Thus, on square lattices, one should need exceptionally low growth temperatures to fabricate noncompact islands. In contrast, our variable temperature scanning tunneling microscopy measurements of Cu growth on Ni(100) reveal that islands with noncompact shape occur on surfaces with square symmetry at surprisingly high growth temperatures (250 - 370 K). The underlying physical mechanism is the preferential strain relief (2.6 % compressive strain) at step edges. Above a critical island size of about 200 atoms there is a high probability for the islands to become noncompact in order to optimize the ratio between perimeter and surface. The noncompactness of islands is quantified by the Hausdorff dimension, which is measured to be 1.7. The quantitative analysis of the growth of noncompact islands reveals an unusual coalescence behavior and a fundamental broadening of the scaled island size distribution.

P-25

Diffusion of Copper Adatoms on Cu(111) Surface by Molecular Dynamics Simulation. N. PAPANICOLAOU, Dept. of Physics, University of Ioannina, P.O. Box 1186, GR-45110 Ioannina, Greece. - - - The self-diffusion process of single adatoms on the Cu(111) surface has been studied using molecular dynamics simulation and a n-body potential adapted to copper. From the detailed analysis of adatom trajectories we have deduced the diffusion coefficient, which exhibits Arrhenius behavior, along with the corresponding migration energy. In addition we have found a new hopping mechanism, which explains the existing discrepancies concerning the adatom's migration energy. The associated energies compare well with the available experimental data.

P-26

Simulations of Small Polar Molecules on Oxide Surfaces. D. PASCHEK and A. Geiger, University of Dortmund, 44221 Dortmund, Germany. - - - A realistic model of molecularly adsorbed ammonia on the (110) surface of TiO₂ (rutile) has been studied by means of Molecular Dynamics. The simulations were carried out within a temperature range between 100 K and 450 K. The complex behavior of the translational dynamics was attributed to the specific structure of the substrate and has been characterized as an 'exchange reaction' between two distinct adsorbed states on the surface. The high lateral mobility of weakly bound 2nd layer molecules leads to rapid isotropic diffusion on the surface of micro-crystalline powders and thus serves as an explanation for the experimentally obtained singulett peak in ²H-NMR spectra.

P-27

Surface Diffusion on Correlated Heterogeneous Substrates. A. Ramirez Cuesta, F. Bulnes, F. Nieto, M. Nazzarro, J. Ramirez Pastor, and V. PEREYRA, Departamento de Fisica, University of San Luis, Chacabuco 917, San Luis 5700, Argentina. - - - The collective motion of particles on a generalized heterogeneous surface is studied by means of Monte Carlo simulation. Using the dual site-bond model(SBM), the energetic properties of the heterogeneous substrates can be appropriately described through the site and the bond energy distributions and the overlapping degree between them. The effect of the adsorptive energy topography on the tracer diffusion coefficient, thermodynamical factor and consequently the collective diffusion coefficient is analyzed for different coverage, temperature and energy correlation degrees. We observe that the short-time behavior of the mean-square displacement is highly sensitive to the surface energy structure. The condition under which the temperature dependence of the tracer diffusion coefficient shows a non-arrhenian behavior is discussed. Surface diffusion emerges as an important tool for the characterization of the energetic topography on heterogeneous surfaces.

P-28

Temperature Dependence of the Diffusion Coefficient on Dynamical Random Barrier Model. F. Bulnes, F. Nieto, and V. PEREYRA, Departamento de Fisica, University of San Luis, Chacabuco 917, San Luis 5700, Argentina. - - - It is well known that temperature dependence of the diffusion coefficient on Random Barrier Model is determined by the coordination number z of the lattice for frozen barrier disorder. On a hypercubic lattice it is of Arrhenius form and for $z > 4$ it deviates from it with increasing degree of disorder. In case of the dynamically changing disorder, whereby the random environment is renewed with a given frequency, the temperature behavior of the diffusion coefficient D is always non-Arrhenia. We use lattices with randomly "dynamically" distributed barrier energies to study diffusion properties as a function of the temperature and disorder degree. By means of standard Monte Carlo techniques we analyze the movement of a particle on such disordered medium. the transition characteristics are governed by Boltzman statistics. Our results shown that the temperature behavior of D present a crossover between the classical Arrhenian and a power-law dependence at low temperature.

P-29

Surface Diffusion of Dimers on Different Substrates. A. J. Ramirez Pastor, M. Nazzarro, J. L. Riccardo, and V. PEREYRA, Departamento de Fisica, University of San Luis, Chacabuco 917, San Luis 5700, Argentina. - - - We analyze the diffusion process of asymmetrical dimer (AB) on different substrates by means of Monte Carlo simulation. The coverage dependence of the collective diffusion coefficient is obtained by using of the Green-Kubo method. Different adsorbate-adsorbate interactions (AA, AB, BB) are considered in order to analyzed the influence of such parameters on the diffusion process. We studied the behavior of the diffusion coefficient in the critical region, where several ordered adsorbate structures appear depending on the values of the adsorbate-adsorbate interactions. Stepped and patchwise surfaces are introduced to analyze the influence of the surface geometry on the dimer diffusion process.

Surface Diffusion of 3d-Metals on W(110). D. REUTER, Max-Planck-Institut
Für Mikrostrukturphysik, AM Weinberg 2, D-06120 Halle/Saale, GERMANY. - - -

We studied the surface diffusion of Fe, Ni, Co and Cu on W(110) in the temperature range from 670 K to 1070 K. By evaporating through a mask with a hole we prepared a metal dot on the tungsten surface. After annealing the sample we studied the diffusion behavior of the material with Scanning Auger- and Scanning Electron Microscopy. We observe for all four metals anisotropic diffusion. For Fe, Co and Ni a one monolayer (ML) thick film spreads over the substrate surface ("unrolling carpet mechanism"). For Fe the direction of fast diffusion is determined by the crystallographic structure of the substrate surface (fast direction along $\langle 1-10 \rangle$), whereas for Ni the local nanostructure (probably density and direction of steps) has a strong influence on the diffusion behavior. Co shows a temperature depended anisotropy. For low temperatures (< 870 K) the local nanostructure determines the direction of fast diffusion, whereas for higher temperatures the fast direction lies along the $\langle 1-10 \rangle$ -direction of the substrate surface.

For Cu we observe the simultaneous spreading of a 2 ML and a 1 ML thick film. The anisotropy for the first ML is determined by the local nanostructure of the substrate surface, whereas the direction of fast diffusion for the second ML is along the $\langle 001 \rangle$ -direction of the W(110)-surface.

Sites and Mobility of Isolated In-111 Atoms After Low Energy Deposition on Stepped Cu(100) Surfaces. M. F. ROSU, Nuclear Solid State Physics, Rijks Universiteit Groningen, Nijenborgh 4, 9747 AG Groningen, GERMANY. - - - We measured atomic sites of isolated In-111 atoms after deposition at 80K on a stepped Cu(100) surface, using the perturbed angular correlations technique. The influence of the deposition energy on the as-deposited In environments was investigated for energies ranging from ~5 to 50 eV. An isochronal annealing program was performed in order to study the subsequent diffusion of the In atoms over the stepped surface.

We find that up to energies of about 5 eV, the In probes are exposed to two unique and highly symmetric environments, similar to the ones measured after evaporation of In-111 probes. These sites were attributed by Fink et al.¹ to adatomic and adatomic step (kink) sites, respectively. After annealing to 100 K the In atoms initially located at adatomic terrace sites have diffused to the Cu steps, and are probably trapped at kink sites. After annealing to about 160 K the In atoms have diffused into the step, while after annealing to 300 K the majority of the In atoms are located at substitutional terrace sites.

At an deposition energy of 15 eV at 80 K, the above two adatomic sites have completely disappeared and the large majority of the In atoms are located at well defined substitutional terrace sites and substitutional step sites.

The results are compared to Molecular Dynamics simulations of the deposition process, using modified Finnis-Sinclair potentials to describe the interatomic interactions.

¹R. Fink. . .

P-32

Dissolution Kinetics of a Thin Metal Deposit on a Metallic Substrate: Ag/Cu and Ni/Ag. A. SAUL, Campus de Luminy, Case 913, 13288 Marseille Cedex 9, FRANCE. - - - The kinetics of dissolution of one layer of an A metal deposited on a B substrate is strongly influenced by the energetic forces which drive equilibrium surface segregation in the corresponding A_cB_{1-c} alloy. Modeling this process by a Kinetic Tight Binding Ising model, either using a mean-field or a Monte Carlo approach, allow us to predict a wide variety of dissolution modes, the nature of which strongly depends on the tendency of the AB system to order or phase separate in the bulk.

When there is a preference for the formation of homoatomic AA and BB pairs, one predicts either the existence of a new layer-by-layer dissolution mode (analogous to the layer-by-layer growth mode) when the deposited element tends to segregate (Ag/Cu) or the encapsulation of the deposited film below one or two floating substrate layers, before its dissolution in the reversed case (Ni/Ag).

P-33

Theoretical Estimation of Atomic Positions in the Surface Layers of Low Index Planes of Al. P. SCHAROCH, J. Peisert, Institute of Physics, Wroclaw, Technical University, Wroclaw, Poland, A. Kiejna, Institute of Experimental Physics, University of Wroclaw, Wroclaw, Poland. - - - The experimental investigations demonstrate that the positions of atoms in a surface layers of solids are relaxed compared to their positions in the bulk. Using the local density-functional theory and the 'ab initio' pseudopotential formalism we have determined the positions of atoms in the topmost layers of low-index planes of aluminum. The surfaces are modeled by supercells. The electronic ground state is determined by minimizing the electronic free energy in the Car-Parinello-like iterative way. Simultaneously, the atomic structure is optimized using damped dynamics.¹ The results obtained are in a good agreement with the measured values.

¹R. Stumpf and M. Scheffler, *Comput. Phys. Commun.* **79**,447(1994).

P-34

Collective Diffusion in Adsorbates with Dipolar Lateral Interactions. A. Danani, R. Ferrando, E. Scalas, Università di Genova, Italy and M. TORRI, Department of Physics, University of Alberta, T6M 2J1 - Edmonton, Canada. - - - Collective diffusion in adsorbates in the presence of long-range dipolar lateral interactions is studied in terms of a kinetic lattice-gas model. The model is treated in the framework of the Mori projection-operator technique. An exact expression for the average jump rate as a function of the coverage is derived. The two-points static correlations in the lattice gas are calculated using the Hypernetted Chain Equation. Higher orders static correlations are obtained in the Kirkwood approximation. The diffusion coefficient is computed in the Darken approximation for a wide range of coverages and temperatures. The model can be relevant in the case of alkali metals, adsorbed on transition metals, such as Na on Cu.

P-35

Resonant Diffusion on Solid Surfaces. R. TSEKOV, Department of Physical Chemistry, University of Sofia, Sofia, Bulgaria. - - - A new stochastic approach to Brownian motion of atoms and atomic clusters on solid surfaces is developed. The main problem discussed is the dependence of diffusion coefficient on the fitness between the surface static potential and the internal cluster configuration. It is shown that this dependence is non-monothonic which is the essence of the so-called resonant diffusion. Assuming internal motions of the cluster much more quicker than its translation, adiabatic separation of these variables is possible and a relatively simple expression for the diffusion coefficient is obtained. In this way, the role of cluster rotation is accounted for, thus leading to more complex resonances in the cluster surface mobility.

P-36

Domain Growth kinetics with Conserved Dynamics. M. VELGAKIS, University of Patras, 26500 Patras, Greece. - - - The dynamical properties of model systems with spin-exchange kinetic dynamics are investigated by means of computer simulations. These systems serve to simulate diffusive processes in solids and are well suited to reveal the basic features of kinetic phenomena near equilibrium. Diffusion of tracer particles in interacting lattice gases is studied. The time-dependent of the diffusion coefficient has been derived and the analogies to the relaxation in disordered systems, such as the a:Si-H, are also discussed.

Diffusion of Interacting Lattice Gases on Heterogeneous Surfaces with Simple Topographies. C. UEBING, Max-Planck-Institut fuer Eisenforschung, Postfach 140444, D-40074 Duesseldorf, Germany, V. PEREYRA, Departamento de Fisica, Universidad Nacional de San Luis Chacabuco 917, 5700 San Luis, Argentina. - - -

The study of collective surface diffusion of adsorbed molecules on solid surface has been a subject of increasing interest in the last decades due to the importance of this phenomenon in many surface molecular processes, like adsorption and gas separation, catalysis, film growth, etc., and to the fact that the development of new and better experimental techniques stimulates the need for a better understanding of the surface diffusion from a microscopical point of view. Surface diffusion has been most extensively studied for homogeneous surfaces, where the influence of adsorbate-adsorbate interactions and phase transitions has been deeply investigated. However, real solid surfaces are generally heterogeneous and the study of heterogeneity effects on surface diffusion coefficients is of capital importance. In the present work we have studied the diffusion of interacting and non-interacting lattice gases on heterogeneous bivariate trap surfaces with different topographies. The topography is shown to affect strongly the coverage dependence and Arrhenius behavior of diffusion coefficients. The fluctuation and Kubo-Green methods are used for the determination of the collective diffusion coefficient. Both methods reveal numerically different results, which is attributed to the failure of the former when the probe-size is of the order of the applicable scale length for the lattice gas.

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P-38

Inter-Layer Diffusion in a Submonolayer, Low Island Density Regime During Epitaxial Growth. K. R. ROOS, Bradley University, Department of Physics, Peoria, IL 61625. - - - We use Monte Carlo simulations to study inter-layer mass transport during submonolayer epitaxial growth in systems where the ratio of D (the diffusion coefficient for intra-layer diffusion) to F (the deposition flux) is very high. Under these growth conditions, because of the presence of finite-sized terraces there exists a low island density regime where the scaling relation, between the island density and the ratio D/F , from nucleation theory breaks down. We employ realistic terrace boundaries in our simulations, including an additional barrier height (above the on-terrace diffusion barrier) to diffusion at a descending terrace edge, and we investigate the D/F dependent inter-layer diffusion in the low island density regime. An activation energy can be extracted from the growth rate of the few islands in this regime and we show that this activation energy can be directly related to the terrace edge barrier to inter-layer diffusion.

P-39

Formation of New Terraces via Diffusion Induced by the Field Gradient in STM. J. MENDEZ, J. GOMEZ-HERRERO, and A. M. Baro, Lab. Nuevas Microscopias, Dept. Fisica de la Materia Condensada, Universidad Autonoma de Madrid, 28049 Madrid, SPAIN. - - - The possibility of creating new terraces on a metal surface is demonstrated. Using a single crystal of Au (110) as substrate and a STM's tip as a tool, we induce adatoms of gold to form new terraces under the tip. The mechanism is directional diffusion induced by the electrical field gradient. The formed terraces show clear (1×2) reconstruction indicating that the nature of these terraces is unequivocally gold.

P-40

Surface Diffusion in Presence of Two Non-Equivalent Lattice Sites in Hexagonal Structure in (111) Direction. M. MASIN and Michal Ondrejcek, Institute of Physics, Czech Academy of Sciences, Prague 6, Czech Republic. - - - The surface diffusion is studied on the two centre fcc structure in (111) direction. The object of our work is determination of the coverage dependence of the diffusion coefficient. Direct interactions between adatoms aren't involved in this model. The simultaneous occupation of nearest neighbor positions is prohibited. Chemical diffusion coefficient is divided into two parts - jump diffusion coefficient and thermodynamic factor, which are determined within the statistical methods. It was shown that the strong dependence of the diffusion coefficient on coverage follows naturally from this model, although direct adatom interactions are excluded.

The results will be compared with the experimental results of surface diffusion of K on Pd(111)¹ and follow the theoretical work [2], that studied surface diffusion in the presence of two non-equivalent lattice sites on fcc in (100) direction.

Reference

¹M. Ondrejcek, W. Stenzel, H. Conrad, V. Chab, Z. Chvoj, W. Engel, and A. M. Bradshaw, *Chem. Phys. Lett.* **215**, 528 (1993).

²Z. Chvoj, H. Conrad, V. Chab, M. Ondrejcek, and A. M. Bradshaw, *Surf. Sci.* **329**, 121 (1995).

P-41

Self-diffusion on Ni(110) Studied by He Atom Scattering, Walter SILVESTRI, Max-Planck-Institut für Stroemungsforschung, Goettingen, Germany. - - - The self-diffusion of Ni on Ni(110) has been studied by He atom scattering. The quasi-elastic peak was analysed by deconvolution techniques and thus the broadening of the peak, due to moving atoms on the surface was calculated. From this the diffusion coefficient was obtained. The activation energies and k-space dependence were thus measured along several directions.

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