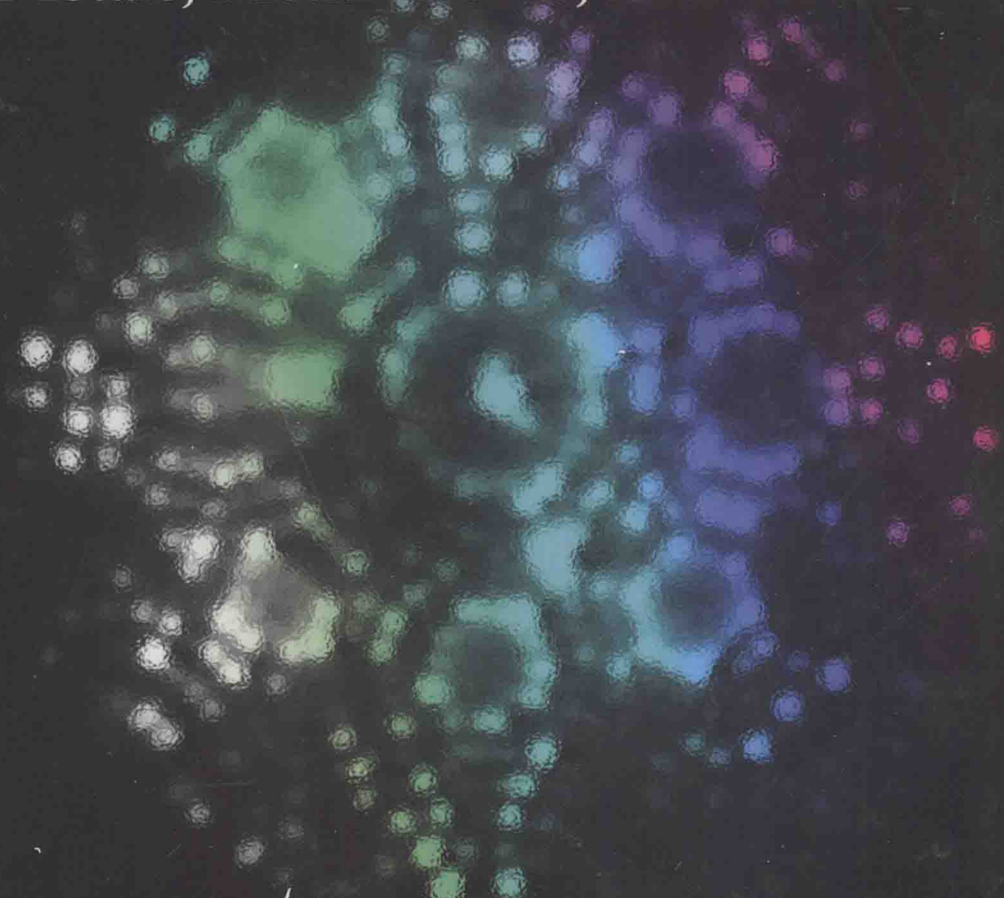
Surface Diffusion

Metals, Metal Atoms, and Clusters



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Surface Diffusion

Metals, Metal Atoms, and Clusters

For the first time, this book unites the theory, experimental techniques, and computational tools used to describe the diffusion of atoms, molecules, and nanoparticles across metal surfaces. Starting with an outline of the formalism that describes diffusion on surfaces, the authors guide the reader through the principles of atomic movement, before moving on to describe diffusion under special circumstances, such as the presence of defects or foreign species. With an initial focus on the behavior of single entities on a surface, later chapters address the movement of clusters of atoms and the interactions between adatoms. While there is a special emphasis on experimental work, attention is paid to the increasingly valuable contributions theoretical work has made in this field. This book has wide interdisciplinary appeal and is ideal for researchers in solid state physics and chemistry, as well as materials science and engineering.

Grażyna Antczak is a Humboldt Fellow in the Solid State Physics Department at Leibniz University, Hannover, Germany. She received her Ph.D. from the Institute of Experimental Physics at the University of Wrocław, Poland, where she is now an adjunct researcher. Dr. Antczak is a Member of the American Physical Society and the American Vacuum Society, and has had 15 publications in scientific journals.

Gert Ehrlich is currently Research Professor in the Department of Materials Science and Engineering at the University of Illinois, Urbana-Champaign. He is internationally recognized as a pioneer in the area of surface diffusion, and he has received numerous scientific honours and awards. Dr. Ehrlich is an active member of various societies, and is a Fellow of the American Physical Society and the New York Academy of Sciences. He has written almost 200 journal articles and has served on several editorial advisory boards.

Preface

Surface diffusion on metals has been a subject of scientific interest for roughly ninety years. During the first forty years of this period it was very hard to do meaningful work because of technical problems – the difficulty of establishing good enough vacuum conditions to maintain a surface clean for measurements. In a few laboratories, mostly industrial, ultrahigh vacuum techniques were already practiced at that time, but this was not the normal course of events. All of this changed after World War II, first with the general adoption of good vacuum practices, and then with the development of more capable techniques for examining kinetic processes that are important on a surface. The first of these techniques was field ion microscopy, invented by Erwin Müller [1,2], the first method to provide a direct view of single atoms on a surface. The next important development was the scanning tunneling microscope, devised by Binnig and Rohrer [3], which established the capability of probing a large scale surface with high resolution. The last major contribution was the progress in theoretical techniques and computer technology, which toward the end of the twentieth century led to the rapid growth of theoretical calculations.

The last forty years have therefore been a time of great progress in our understanding of surface diffusion, especially of metal atoms on metals. These advances have been spread over the scientific literature, and there has been no overview of the entire field, which is what we are trying to provide here. Our primary emphasis will be on experimental work to define the processes participating in surface diffusion. However, theoretical work can now be done so expeditiously that it has provided valuable guidance, and is now being intensively pursued. As such these contributions will also be carefully noted.[1] Surface diffusion has, of course, a long history, dating back to the initiating work of Hamburger [5] in 1918. These early studies have, however, already been reviewed [6], so here we will be concerned with work on surface diffusion under ultra high vacuum (UHV) conditions and on an atomic scale, which began in the 1960s, and has led to the current state of understanding.

The beginnings of modern studies of surface diffusion were greatly influenced by the insights and inspiration of David Turnbull, as well as by the traditions and expertise at General Electric. We have also benefited from the encouragement and suggestions of Ryszard Błaszczyszyn, and were able to draw on the expertise at the Institute of Experimental Physics of the University of Wrocław. Here, at the University of Illinois,

[1] For a review of theoretical efforts, see T. Ala-Nissila *et al.* [4].

we have had helpful interactions with Dan Alpert, the man that guided the start of modern ultrahigh vacuum techniques which underlie diffusion studies on surfaces. Above all, GE wants to express his appreciation to his wife for her support and for the time devoted to this effort.

The point of view of this presentation is primarily atomistic, and this was stimulated by the work of J. H. de Boer in his book *The Dynamical Character of Adsorption*, Clarendon Press, Oxford 1953, which had quite an impact on us. It is important to recognize that the term surface diffusion spans topics much broader than what we intend to cover here. Our concern will be concentrated on the behavior of single entities and clusters on a surface. This avoids encountering the interactions between atoms which affect surface diffusion at finite concentrations, and are specific to the particular chemistry of each system. However, with an understanding of surface diffusion gained from experiment and theory, work on interactions between adatoms will be described as well.

Our efforts have greatly benefited from interactions with the various members of the Surface Studies group here over the years, and we express to them our great appreciation. We also want to emphasize again the crucial importance of experimental work, and of the technical support necessary for this. It is therefore a pleasure to give our thanks to the people who primarily provided this support for us: Bob Bales, Jack Gladin, William Lawrence, and Bob MacFarlane. Also important in coming to grips with the subject of surface diffusion was the assistance of Mary Kay Newman, the librarian in the Physics Department, whose help, as well as that of Nicholas Watanabe, has been really appreciated. Finally we want to acknowledge a special debt to Jennifer Lewis, who made it possible for us to continue our work.

References

[1] E. W. Müller, K. Bahadur, Field ionization of gases at a metal surface and the resolution of the field ion microscope, *Phys. Rev.* **102** (1956) 624–631.

[2] E. W. Müller, T. T. Tsong, *Field Ion Microscopy Principles and Applications* (American Elsevier, New York, 1969).

[3] G. Binnig, H. Rohrer, Scanning tunneling microscopy, *Helv. Phys. Acta* **55** (1982) 726–735.

[4] T. Ala-Nissila, R. Ferrando, S. C. Ying, Collective and single particle diffusion on surfaces, *Adv. Phys.* **51** (2002) 949–1078.

[5] L. Hamburger, Ultra-microscopic examinations of very thin metal and salt deposits obtained by evaporation in a high vacuum, *Kolloid Z.* **23** (1918) 177–199.

[6] G. Antczak, G. Ehrlich, The beginnings of surface diffusion studies, *Surf. Sci.* **589** (2005) 52–66.

Abbreviations

A	Type *A* step edge on fcc(111)
AES	Auger electron spectroscopy
AFW	Adams, Foiles, Wolfer
Ass	Assigned
ATVF	Ackland, Tichy, Vitek, Finnis
A-Ex	Adatom catalyzed exchange
B	Type *B* step edge on fcc(111)
CEM	Corrected effective medium method
CEM59	CEM with 59 active atoms
CM	Concerted motion
Coh.	Cohesion approximation
COM	Center of mass
COP	Center of positions
CS	Constrained statics
CY-EAM	EAM of Cai and Ye
CY-EAM1	Extension of CY-EAM
CY-EAM2	Extension of CY-EAM
DFT	Density functional theory
Diam	Diameter
DL	Discommensuration line
D-Ex	Double exchange
EAG	Ercolessi–Adams glue potential
EAM	Embedded atom method
EAM5	Embedded atom method 5
EMT	Effective medium theory
Ener min	Energy minimum
Eq.	Equation
Ex	Exchange
FDB	Foiles, Daw, Baskes
FEM	Field electron emission microscopy
FIM	Field ion microscope or microscopy
Fluct	Fluctuation
F-S	Finnis–Sinclair

GGA	Generalized gradient approximation
GP	Glue potential
He-Scat	Helium scattering
^{3}He- SE	^{3}He spin echo
HR	High resolution
HRLEED	High resolution low energy electron diffraction
K	Kelvin
K	Kink
K-K-R	Korringa–Kohn–Rostoker method
LAM	Lonely atom method
LDA	Local density approximation
LDOS	Local density of states
LEED	Low energy electron diffraction
LEEM	Low energy electron microsopy
LEIS	Low energy ion scattering
L-Ex	Long exchange
LF	Leapfrog
LMD	Langevin molecular dynamics
L-J	Lennard Jones
Mag	Magnetic
MAEAM	Modified analytical embedded atom method
MC	Monte Carlo
MD	Molecular dynamics
MD/MC-CEM	Molecular dynamics/Monte Carlo using CEM
MBE	Molecular beam epitaxy
ML	Monolayers
Morse	Morse potential
MS	Molecular statics
MW	Metastable walk
M-Jump	Meta jump
NEB	Nudged elastic band
nn	Nearest neighbor
Nucl	Nucleation theory
OJ	Oh and Johnson
PACS	Perturbed $\gamma - \gamma$ angular correlation studies
PEEM	Photoemission electron microscope
Photo	Photoemission
Pot	Potential
RD	Ring diameter
Rean	Reanalyzed
Refit	Refitted and reanalyzed
Resis	Resistivity
RGL	Rosato, Guillope, Legrand

RHEED	Reflection high energy electron diffraction
RS	Rutherford scattering
SC	Sutton–Chen
Scat	Scattering
SEAM	Surface embedded atom method
SEM	Scanning electron microscope
SI	Surface ionization
sim	Simulation
SPA-LEED	Spot profile analysis of low energy electron diffraction
Static	Static barrier
STM	Scanning tunneling microscope or microscopy
T	Temperature
TB	Tight-binding
TDT	Tersoff, Denier van der Gon, and Tromp
TI	Thermodynamic integration
TST	Transition state theory
T-Ex	Triple exchange
Q-Ex	Quadruple exchange
VASP	Vienna *ab initio* simulation package
VC	Voter Chen
VTST	Variational transition state theory
WF	Work function
XPD	X-ray photoelectron diffraction
XPS	X-ray photoelectron spectroscopy
Z	Band occupation
$\parallel$	In-channel
$\perp$	Cross-channel

Symbols

α	Jump rate to nearest-neighbor position at the right for 1D motion, or jump rate to nearest-neighbor position for 2D motion
α_{fh}/α_{hf}	Rate of single jumps from fcc to hcp/hcp to fcc site on fcc(111)
α_M	Morse parameter
α_N/α_L	Exponent describing dependence of diffusivity D on number of atoms N/on radius of island R_r, or island of length L_L
α_{Re}	Rate of short range mechanism of movement for Re-Ir complex
a_ℓ	Lattice spacing
a_S	Atom jump rate along step of type A
A	Island area
A_R	Parameter of repulsive energy
β	Jump rate to next nearest-neighbor position at the right for 1D motion, or jump rate to next nearest-neighbor position for 2D motion
β_{ff}/β_{hh}	Rate of double jumps between fcc/hcp sites on fcc(111)
β_{R}	Jump rate for rebound jumps
β_{Re}	Long range mechanism of movement for Re-Ir complex
b_S	Atom jump rate along step of type B
χ_{c}	Energy of condensation on fcc(111) plane
c	Concentration, or rate of dimer jump via horizontal intermediate on bcc(110)
c_0	Concentration at $t = 0$
δ	Jump rate to nearest-neighbor position at the left in 1D movement
δ_F	Fermi-level phase shift
δ_D	Distance between interior and step edge barrier
δ_{xo}	Kronecker delta
δ_x/δ_y	Rate of horizontal/vertical jump on bcc(110)
d_d	Distance
d_{12}	Separation of atom 1 and 2
d_t	Rate of adatom motion on terrace
d_T	Trio perimeter
d_R	Plane diameter
D	Diffusivity
D_o	Prefactor of the diffusivity

D_{0B}	Prefactor of diffusivity over descending step
D_M	Morse parameter
D_{205}	Diffusivity of cluster consisting of 205 atoms
D_γ	Diffusivity calculated with all types of jumps
D^*	Prefactor in diffusivity dependence on cluster size
ε	Jump rate to next-nearest-neighbor position at the left in 1D movement
ε_{LJ}	Energy parameter of L-J potential
$\varepsilon_1/\varepsilon_2/\varepsilon_3$	First/second/third nearest-neighbor pairwise interaction
ε_F	Fermi energy
ε_{R}	Repulsive pair energy
ε_{AA}	Interaction energy between two similar atoms at nearest-neighbor sites
$\varepsilon_{xx}/\varepsilon_{yy}$	Strain
e	Charge of the electron
E^A/E^B	Activation energy for movement along step *A*/step *B*
E_2^{sh}/E_2^{st}	Barrier for dimer shearing / stretching
E_B^i	Band energy
E_D^D/E_D^v	Activation energy for movement obtained from diffusivity/velocity
E_R^i	Repulsive energy between two atoms
E_{ℓ_0}	Energy of two adatoms at nearest-neighbor separation
E_1	Energy of dimer in configuration 1, or binding energy for adatoms at *nn* separation
E_2/E_3	Binding energy for adatoms in second/third *nn* separation
E_0	Energy of dimer in configuration 0
$E_{\alpha f}/E_{\alpha h}$	Barrier height for jump out of fcc/hcp site
$E_\alpha/E_\beta/E_{\beta R}$	Activation energy for single/double/rebound jumps
$E_{\delta x}/E_{\delta y}/E_s$	Activation energy for vertical/horizontal/sum of jumps
E_a	Additional step-edge barrier, or activation energy for jump *a* in dimer movement
E_b	Activation energy for jump *b* in dimer movement
E_{cb}	Energy of core break up
E_{cc}	Energy of new row nucleation
E_{coh}	Cohesive energy
E_{CJ}	Activation energy for concerted jump
E_e/E_h	Barrier for exchange/hop
E_{eff}	Effective energy barrier
E_e^A/E_e^B	Activation energy for exchange along step *A*/step *B*
E_h^A/E_h^B	Activation energy for jump along step *A*/step *B*
E_i	Cluster binding energy, or internal energy due to atom *i*
E_j/E_ℓ	Activation energy for *j*-/ℓ-type long jump
E_{ij}	Potential energy between atoms *i* and *j*
$E_{ij,\ell}$	Energy of two atoms at sites *i* and *j* in state ℓ

E_k	Energy of adatom pair in configuration k
E_{kd}/E_{ku}	Energy of down jump/up jump at kink
$E_{b\ell}$	Activation energy for conversion from single to ℓ-type long jump
E_B	Activation energy for overcoming descending step and incorporate
E_{B2}	Activation energy for overcoming descending step at B_2 position and incorporate
E_{He}	Incident energy of helium
E_{LF}	Activation energy for leapfrog event
E_p	Energy of movement along step
E_r	Rebound energy
E_T	Activation energy for diagonal transition around cluster corner
E_{tot}	Total energy
$E(a,b)$	Energy of atom pair at separation $\boldsymbol{R}=(a,b)$
$E(d)$	Pair interaction energy at separation d
$E(s)$	Energy as a function of the displacement s
ΔE	Energy change
ΔE_a	Effective energy for movement of cross-channel dimer from state 0 to state 1
ΔE_b	Effective energy for movement of cross-channel dimer from state 1 to state 0
ΔE_{cs}	Binding energy of core atom relative to adatom at step
ΔE_D	Energy of activation for diffusion
ΔE_ε	Energy width in time of flight spectrum
ΔE_e	Activation energy for cluster movement by atom exchange
ΔE_h	Activation energy for cluster movement by atom hopping
ΔE_{int}	Interaction energy
ΔE_{ks}	Binding energy of kink atom
ΔE_{kt}	Binding energy of kink atom relative to atom on terrace
ΔE_{vib}	Vibrational contribution to energy of activation
$\Delta E(\varepsilon)$	Energy changes during collision
$< E_T >$	Mean kinetic energy
$< \Delta \mathrm{E} >_{\mathrm{AT}}$	Effective activation energy for atomic motion of dimer
$< \Delta \mathrm{E} >_{\mathrm{COM}}$	Effective activation energy for center of mass motion of cluster
ϕ	Electron work function
$\phi_{ij}(R_{ij})$	Core–core repulsion between atoms i and j
$\Delta\Phi$	Difference in structural energy between barrier peak and normal position
$f_i(t)$	Auto-correlation function for electron emission fluctuation
$f_j(R_{ij})$	Contribution of electron density of atom i arising from atom j
F	Free energy
F_a	Force
F_e	Electric field
F_f	Rate of atom deposition

F_x	Free energy for atoms x units apart
$F(a,b)$	Free energy of atom pair at separation $\boldsymbol{R} = (a,b)$
$F(\boldsymbol{R})$	Free energy of interaction as a function of the separation $\boldsymbol{R}$
$F(t)$	Fraction of atoms on the surface
$F_i(\rho_i)$	Energy for embedding atom into local density ρ_i
ΔF	Free energy change
ΔF_D	Change in free energy for diffusion
γ	Jump rate to third neighbor position
$\gamma - \gamma$	Angular correlation
γ_s	Formation energy per step atom
Γ	Jump rate
Γ_o	Prefactor for the jump rate
Γ_i	Rate of dissociation of island of size i
Γ_ε	Quasielastic energy width of scattered atoms
g	Geometrical factor
$g(\boldsymbol{R})$	Pair distribution function
$G(t,z)$	Moment generating function of variable z
h	Planck's constant
h_a	Rate of detachment of atom adsorbed at straight edge
h_c	Rate of core breakup
h_e	Rate of straight edge hopping
h_k	Rate of kink escape
h_{ke}/h_{se}	Rate of detachment of atom from kink/from straight edge to terrace
h_r	Rate of conversion of vertical to horizontal dimer, or rate of corner rounding
h_{re}	Rate of detachment of atom from corner to the step edge
H_s^o	Enthalpy of sublimation
$\hbar$	$\frac{h}{2\pi}$
i	Critical size of cluster
I	Ionization potential
I_e	Density of the emission current
I_{exp}	Intensity of scattered He atoms
I_{fit}	Best model fit to scattered He atom intensity
I_R	Kinematic RHEED intensity
$\frac{I}{I_0}$	Ratio of scattered to incident intensity
$I_n(\tau)$	Modified Bessel function of order n and argument τ
j	Flux across unit length of line
j_B	Atom jump rate over barrier E_B at step edge
j_D	Diffusive flux
j_R	Flux at position R
κ	Ratio of force constants

k	Boltzmann's constant
k_h	Harmonic approximation of escape rate
k_a / k_{ke}	Rate of atom attachment from terrace to straight step/to kink
k_k	Rate of atom attachment from edge to kink
k_{force}	Force constant
k_F	Fermi wave number
λ_{deB}	deBroglie wave length
λ_F	Fermi wave length
λ_x	Jump rate to right, starting from position x
ℓ	Jump length, or quantum state
ℓ_0	Nearest-neighbor spacing
L	Number of sites in one-dimensional plane
L_0	Standard length
L_i	Island separation
L_L	Island length or diameter also side length of square deposit
L_T	Tip to detector distance
μ	Chemical potential
μ_x	Jump rate to left, starting from position x
m	Mass of electron
m_a	Number of deposited atoms, or number of atoms adsorbed per cm^2
m_1, m_2	Number of atoms per unit length
M	Number of atoms adsorbed, or total number of observations
M_S	Number of surface sites
M_T	Magnification of field ion microscope
ν	Attempt frequency of atom
ν_0	Frequency prefactor for diffusion
ν_s	Frequency prefactor for diffusion across descending steps
ν_h	Harmonic approximation attempt frequency for diffusing adatom
$\nu_{0\alpha}/\nu_{0\beta}/\nu_{0\beta R}$	Prefactor for single/double/rebound jumps
$\nu_\alpha/\nu_r/\nu_{ce}/\nu_{all}$	Frequency of single/reinsertion/correlated / all jumps
$\nu_{0\delta x}/\nu_{0\delta y}/\nu_{0s}$	Prefactor for horizontal/vertical/sum of jumps
ν_{0B}	Frequency factor for descending lattice step
ν_a	Relative frequency factor of step edge to terrace diffusion, or frequency for rate a in dimer motion
ν_b	Frequency for rate b in dimer motion
ν_d	Frequency factor
ν_ℓ/ν_j	Frequency factor for ℓ-/j-type jumps
$\nu_{b\ell}$	Frequency factor for conversion from single to longer jump
n	Number of jumps
n_x	Number of islands per site
n_c	Number of charges on the evaporated ion
n_{out}/n_{in}	Number of paths for going out/in over boundary
$\langle n \rangle$	Number of diffusion events

N	Number of atoms in cluster, size of island, or total number of transitions (jumps)
N_a	Number of atoms simulated
N_{av}/N_{av}^0	Mean island density/initial post-deposition mean island density
N_I/N_{II}	Frequency of occurrence of island in form *I*/form *II*
N_c	Number of atoms in hexagonal form
N_f/N_h	Number of atoms at fcc/hcp sites
N_i/N_t	Number of atoms incorporated/trapped
$N_{\alpha f}/N_{\alpha h}$	Number of hops out from fcc/hcp site to the same kind of site
N_T	Total number of jumps
$N(\boldsymbol{R})$	Number of observations of two atoms separated by $\boldsymbol{R}$
$N_o(\boldsymbol{R})$	Total number of atom pairs at separation $\boldsymbol{R}$
$\overline{N}$	Average number of atom jumps
$<\Delta n_1^2>$	Mean-square value of jumps to the right
p	Probability of jump to the right
$p(\boldsymbol{R})$	Probablility of finding adatom pair at separation $\boldsymbol{R}$
$p_{b\ell}$	Probability of converting from single to long jump
p_{n_1}	Probability of reaching $x = s\ell$ after n_1 jumps
p_x	Probability of atom being at the distance x
$p_{\Delta x}N$	Number of atoms at displacement Δx
P	Probability that material present at $t=0$ will be gone at time τ
P_0/P_1	Probability of being at a site of type 0/type 1
$P_0^{(z)}$	Probability of center of mass being at site of type 0 having started at z
P_{0A}	Probability of finding trimer in configuration *0A*, regardless of position
P_{1D}/P_{2D}	Probability of cluster in 1D/2D configuration
P_b	Probability of atom overcoming step boundary
P_E	Probability of atom occupy edge site
P_{ij}	Probability of finding a pair of atoms at sites i and j
$P(N)$	Term in prefactor for cluster diffusivity accounting for dynamical misfit
$P_f^{(f)}/P_h^{(h)}$	Probablity of atom ending at fcc/hcp site when starting at the same kind of site
θ	Fractional occupation of sites
Θ	Coverage
q	Probability of jump to the left, or distance dependence of hopping integral
q_c	Translational coordinate
q_F	In-surface Fermi wave vector
Q_i	Desorption energy of ion
ρ_i	Electron density of atom i
$\rho(t_f)$	Auto-correlation function
r	Distance between dimer's atoms, or rate of jumps at constant temperature

r_0	Rate of jumps during "zero-time" observations
r_c	Rate of evaporation–condensation mechanism
r_e	Rate of diffusion along cluster perimeter
r_i	Rate of incorpotration to descending step
r_{eq}	Rigid distance between dimer's atoms
r_T	Tip radius
$r1$	Distance of descending step from center
R	Atom deposition rate, or overall rate of jumping
$\boldsymbol{R}$	Adatom–adatom separation vector
$\lvert\boldsymbol{R}\rvert$	Adatom–adatom separation magnitude
R_o	Morse parameter
R_b	Rate of basic jumps, derived from low temperatures
R_c	Cut-off distance for interactions
R_{Fi}	Rate of field ionization
R_ℓ	Rate of long jumps of type ℓ
R_{ij}	Distance between atoms i and j
R_r	Cluster radius or radius of circular deposit
R_s	$\dfrac{E_D}{\Delta H_s^\circ}$
R_T	Tip to screen distance
R_x	Distance from the center of original distribution
R1	Distance of ascending step from center
$<r^2>$	Mean-square displacement in 2D
$<\Delta r^2>$	Fluctuation of displacement in 2D
σ	Interatomic separation at which potential energy vanishes
σ_i	Capture number, relating rate of incorporation to the diffusivity D
σ_x	L-J distance parameter
s	Displacement from initial equilibrium
s_0	Prefactor to $s(T)$
$s(T)$	Ratio of rate of step edge crossing to nearest-neighbor jumps on plane
S_1/S_0	Entropy of dimer in configuration 1/in configuration 0
$\dfrac{s}{s_{tot}}$	Relative distance
S_{av}/S_{av}^0	Mean island size/initial mean island size
ΔS	Change in entropy of system
ΔS_D	Entropy of activation for diffusion
ΔS_{vib}	Vibrational contribution to entropy of activation
τ	Mean lifetime for atom incorporation
τ_0	Prefactor for atom lifetime
τ_c	Lifetime for adatom starting at the center of plane
τ_f	Relaxation time for fluctuation
t_f	Time interval for fluctuation
t	Length of time interval

t_0	Time interval for "zero-time" measurements
t_c	Time interval for diffusion at constant temperature
t_e	Slowly varying functions of $3.79 \times 10^{-4} F_e^{1/2}/\phi$.
T	Temperature
T_d	Temperature for dissociation of cluster
T_D	Temperature for diffusion
T_E	Atom temperature
T_S	Sample temperature
T_m	Melting point
T_R	Temperature for cluster rearrangement
T^*	$\frac{kT}{\varepsilon}$
υ	Correction term in field ionization
υ_e	Slowly varying function of $3.79 \times 10^{-4} F_e^{1/2}/\phi$
v_A	Mean velocity in positive direction
ς	Effective hopping integral, or quarto interactions
v	Velocity
V	Voltage
V_0	Effective barrier for non-interacting atoms
$\langle v_x \rangle$	Average x-component of velocity
ω_0	Angular Debye frequency
ω_d	Angular attempt frequency
$\omega_1/\omega_2/\omega_3$	Frequencies
Ω	Degeneracy
Ω_I/Ω_{II}	Degenerency, number of equal configurations of form I/form II
W	Free energy change between top and bottom of potential
ξ	Mass of an incident compared with a lattice atom
ξ_1/ξ_2	First/second trio interactions
$\langle \Delta x^2 \rangle$	Fluctuation in displacement x
$\langle x^2 \rangle$	Mean square displacement
$\overline{X}$	Mean diffusion length
$X(N)$	Overall displacement
X	Pair separation measured along channel of W(211) plane
y(Å)	Distance perpendicular to step but parallel to surface
$\langle \Delta y^2 \rangle$	Fluctuation in displacement y
$\langle y^2 \rangle$	Mean square displacement
z_A	Partition function of adsorbed material
Z	Canonical partition function
Z_T	Tip sample distance