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MODELING OF THIN-FILM GaAs GROWTH

By

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Progress Report
For the period June 16, 1982 to September 16, 1982

OCT 1982
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NASA STI FACILITY
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September 1982

DEPARTMENT OF MATHEMATICAL SCIENCES
SCHOOL OF SCIENCES AND HEALTH PROFESSIONS
OLD DOMINION UNIVERSITY
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MODELING OF THIN-FILM GaAs GROWTH

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John H. Heinbockel*

SUMMARY

A potential scaling Monte Carlo model of crystal growth is developed. The model is a modification of the solid-on-solid method for studying crystal growth in that potentials at surface sites are continuously updated on a time scale reflecting the surface events of migration, incorporation and evaporation. The model allows for B on A type of crystal growth and lattice disregistry by the assignment of potential values at various surface sites. The surface adatoms are periodically assigned a random energy from a Boltzmann distribution and this energy determines whether the adatoms evaporate, migrate or remain stationary during the sampling interval. For each addition or migration of an adatom, the surface potentials are adjusted to reflect the adsorption, migration or desorption potential changes.

INTRODUCTION

Numerous methods have been applied to obtaining thin-film, single crystals of GaAs, including free-standing wafers, peal films removed from a single crystal substrate, and films grown on lightweight substrates. The most promising method is a version of the latter technique called "graphoepitaxy." It is generally known that overlayers of crystalline materials deposited upon smooth microcrystalline substrates tend to be more or less randomly polycrystalline. The absence of long-range order in the microcrystalline substrate is reflected in the absence of long-range order in the overlayer. The basic concept of graphoepitaxy is that, by introducing an artificial surface relief structure having a long-range order on a microcrystalline substrate, long-range order can be induced in an overlayer. In other words, a crystalline film can be grown on a microcrystalline substrate.

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The degree of crystalline order achieved during a growth process will be controlled by the adsorption, nucleation and lateral growth behavior in the first few deposited layers. The parameters which will affect the crystal growth are: The deposition rate, the surface temperature, surface diffusion, surface defect density and lattice registry of the system. We present a Monte Carlo solid-on-solid (SOS) computer simulation which utilizes a potential scaling technique (ref. 1) over a 20 × 20 array of sites. Although numerous Monte Carlo models for crystal growth exist (refs. 2-12), the approach developed herein is a more physical model in that the events which occur at each site are constrained by the surrounding potential field and the thermal energy fluctations associated with a given substrate temperature. Also, the method of ordered statistics is utilized to construct a time scale of events compatible with computer times in order that the simultaneous changing and updating of site potentials can be done in a reasonable amount of computer time and still allow the model to simulate thin film growth in a physically realistic manner.

LIST OF SYMBOLS

a_0	lattice constant (nm)
M	size of square array
$H(i,j)$	height at position (i,j)
ϕ_0	potential energy change (eV)
ϕ_1, ϕ_2, ϕ_3	first, second, third nearest neighbor potential changes (eV)
ω_i	$(i = 1,\ldots,8)$ potential energy changes (eV)
Δt_s	scanning time interval (sec)
$E(R)$	random energy
$U_0(i,j), U_{os}(i,j)$	potential at site (i,j) for adsorbate and substrate (eV)
$U(i,j)$	total potential at site (i,j) (eV)
U_e, U_{es}	evaporation level of adsorbate and substrate (eV)
U_m, U_{ms}	migration level of adsorbate and substrate (eV)

ϕ^*, R^*, n_o, m_o	Mie potential parameters
K	Boltzmann constant (8.62×10^{-5}) eV/°K
T	absolute temperature (°K)
α_2, α_3	scale factors for crystal orientation
ξ	crystal orientation factors
R	uniform random number $(0 < R < 1)$
R_d	deposition rate (nm/sec)
R_e	evaporation rate
Δt	time interval associated with surface "snapshot"
$\lambda = 1/KT$	parameter of Boltzmann distribution
E	random energy (eV)
$E_{(n)}$	ordered statistic
n	sample size
i,j	site numbers
f(E)	Boltzmann distribution
F(E)	cumulative distribution
g(E)	distribution of ordered statistic E(n)
G(E)	cumulative distribution
(100) (111) (110)	crystal orientations
$\Delta H sub$	heat of sublimation
$\Delta H ads$	heat of adsorption for single adatom
Q_d	diffusion activation energy (eV)
τ	lifetime (sec)
τ_d	mean time between hops
Δt_o	output snapshot or stop action time interval (sec)
U_i	incorporation energy

$U_{ks}^{(1)}$, $U_{ks}^{(2)}$ kink site potentials

m_o, n_o, ϕ^*, R^* Mie potential parameters

D_-, D_+ diffusion coefficients into and from bulk

$S_i = S$ sticking coefficient

τ_o period of vibration of surface atom (sec)

ℓ parameter for surface diffusion

MODELING OF CRYSTAL GROWTH

The SOS Monte Carlo Model

In this model we consider a simple cubic (SC), body centered cubic (BCC) and face centered cubic (FCC) crystal lattice. It is required that each occupied site be directly above another occupied site and so the name solid-on-solid (SOS) model. This model is characterized by an array of interacting columns of varying integer heights with respect to some orientation such as the (100) (111) or (110) crystal planes. The terrace-ledge-kink (Kossel) Model (refs. 13-14) is illustrated in figure 1. The model employs a 20 × 20 square array upon which columns are constructed. Adatoms are deposited upon the surface in a random fashion where they are free to migrate, remain localized, diffuse into the bulk (incorporation) or diffuse from the bulk to the surface, or evaporate. These changes alter the stacking heights of each column as well as producing new potentials at and in the neighborhood of the surface sites involved in the process of surface adatom interaction.

Each surface site is located at the top of the stack of adatoms from an arbitrary row i and column j of a 20 × 20 array. The physical constraints which determine the temporal behavior of every adatom located at the surface of each column from an arbitrary site (i,j) is based upon the interaction potential that the surface adatom has with its nearest neighbors and the rest of the solid. Spatial disregistry, that normally occurs due to size differences between adsorbate and adsorbent atoms, is accounted for by changes in the interaction potential. In figure 2(a), the interaction

potential across a perfectly homogeneous surface is depicted as uniformly changing from site to site. Figure 2(b) illustrates a typical interaction potential across a heterogeneous surface. We developed a set of "rules" whereby the columns of the SOS model interact by assigning values to the potential energy changes associated with the processes of adsorption, migration and desorption.

Potential Scaling of Adatoms

The rules, by which the columns of the SOS model interacted, were governed by the following ideas relating to the potential energy and potential energy changes associated with the adsorption, migration, or desorption of adatoms from an arbitrary row i and column j of an 20×20 array. Energies associated with an arbitrary site (i,j) were defined as follows: $U_0 = U_0(i,j)$--the potential energy at a site because of surface bonding and crystal structure; ϕ_0--the potential energy change at site (i,j) because of the deposition of an adatom (assumed the same for all sites); $-W_i(i = 1, \ldots, 8)$--the potential energy changes at neighboring sites when an adatom is deposited at site (i,j); $E(i,j)$--the random surface energy associated with site (i,j) and time interval Δt_s; $U(i,j) = U_0(i,j) + E(i,j)$--the total energy associated with site (i,j) during the time interval Δt_s; U_e--the evaporation potential; and U_m--the migration potential. All of the above energies are measured in electron volts.

We developed a Monte Carlo computer simulation of crystal growth by developing rules that determined the SOS kinetics of condensation, evaporation or surface migration of adatoms. These rules led to a consistent and physically reasonable description of the fundamentals associated with crystal growth. We first considered the adsorption of a thermally accommodated adatom onto the surface at some general site where the potential at this site was changed and, simultaneously, potential energy changes at all of the neighboring sites occurred. In Table 1, the potential energy changes are depicted by the mnemonic mask. The center of this mask is placed over the site (i,j) to illustrate the changes to be made in the potential at the central site as well as the potential changes in the surrounding neighboring sites.

The potential changes in the case of desorption of an adatom from the central site are again depicted with the mask of Table 1, with the opposite signs on the potential changes. The case of surface migration was treated as a desorption from a site (i,j), followed by an adsorption at a nearest or second nearest neighbor location, together with the correct potential mask changes associated with each process. The neighboring migration site was determined by a weighted random walk to one of the unoccupied neighbor sites.

Table 1. Potential energy changes associated with central site (i,j) and neighbor sites due to deposition of an adatom (for a 100 orientation).

$-w_7 = -w_7(i-1,j-1)$	$-w_8 = -w_8(i-1,j)$	$-w_1 = -w_1(i-1,j+1)$
$-w_6 = -w_6(i,j-1)$	$\phi_0 = \phi_0(i,j)$	$-w_2 = -w_2(i,j+1)$
$-w_5 = -w_5(i+1,j-1)$	$-w_4 = -w_4(i+1,j)$	$-w_3 = -w_3(i+1,j+1)$

The Monte Carlo simulation of crystal growth involved a random deposition of thermally accommodated surface adatoms during a time interval Δt. These deposited adatoms changed the potential energies at the random surface sites under consideration. The values assigned to the central potential change ϕ_0 and neighboring potential changes $-w_i$, $i = 1, \ldots, 8$ dictated the new potential energy values when an adatom was deposited or removed from a site. In this way each surface site had an energy barrier to translation or evaporation, represented by a potential well.

Figure 3 illustrates the potential changes that occur along a lineal section of a homogeneous surface upon the adsorption of a single adatom at site (i,j). Note that the potential increases by an incremental amount ϕ_0, and the adjacent sites decrease in potential by an incremental amount ϕ_1. This represents the actual physical condition that the adsorbed adatom requires less energy to desorb or to migrate as compared to the original surface adatom which was surrounded by all its nearest neighbors. Note also that the deeper potentials at the neighboring sites reflect the increased energy necessary to desorb an atom from these sites due to the increased

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coordination or ligancy created by the adatoms. Figure 4 illustrates the potential variation at an arbitrary site (i,j) as nearest neighbors are progressively added onto a (100) surface orientation.

The term epitaxy means "an arrangement on," and is used to denote the growth of one substance upon the crystal surface of a foreign substance. The term autoepitaxy refers to the oriented growth of a substance onto itself, and hetroepitaxy is the growth over another material. Autoepitaxy requires that the initial potential U_0 (before adsorption) be recovered when the adatom has all its neighboring adatoms surrounding the central site.

In assuming values to the potential changes ϕ_0 and ω_i, i=1,... 8, we must take into account the type of crystal structure and orientation we are trying to simulate with our SOS model. Consider figure 5 which illustrates the GaAs fcc structure. For growth on the (100) face we can set up a correspondence between a central site, the nearest neighbor sites, second nearest neighbor sites, and the adatom potential changes for the mask in Table 1 (i.e., $\omega_1 = \phi_2$, $\omega_2 = \phi_1$, etc.). Similarly, we can set up the correspondence illustrated in figures 5(b and c) for the (111) and (110) orientations and we can construct an appropriate mnemonic mask.

In figure 5 we must choose $\phi_0, \phi_1, \phi_2, \phi_3$ in such a way that, when the first level of adatoms covers the surface, then the potential distribution must return to its original value. We will require that adjustments be made in the potential energy changes during the transition from heteroepitaxy to autoepitaxy. Here we let a negative sign denote an attractive potential. By simply adding adatoms to a surface it is readily verified that the potential changes must adhere to the rules given in Table 2 if after one layer the potential energy returns to its initial value.

For heteroepitaxy we require that an adjustment be made in the central site potential change to reflect the potential energy differences of the materials involved. The potential energy changes $\phi_0, \phi_1, \phi_2, \phi_3$ can be different for the substrate and growing material. For the substrate material we could use the depth of the surface potentials and migration levels to stimulate a variety of surface morphologies. In this model we envision a flat substrate as a periodic lattice structure where each lattice site is a potential well. The substrate can vary from flat to rough and the

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potentials adjusted to reflect various surface preparations. For an ideal
ly flat substrate we assume that the depths of the potential wells are
uniform, given by U_{os}. After one layer of growing material covers the
surface, the potentials at each site are assumed to convert to the auto-
epitaxy potentials U_o. In order to make this transition we assume that

$$\Phi_o = \sum_{i=1}^{8} \omega_i + (U_o - U_{os})\Gamma_{ij}$$ where Γ_{ij} is zero if the height h_{ij} at

position (i,j) is greater than or equal to one, and Γ_{ij} is one in the case
where $h_{ij} = 0$. Thus, if an adatom is deposited at a first layer site
(i,j), we adjust the potentials at this site by the relation $U_o - U_{os}$, in
addition to the mask potential changes at the surface sites as this produces
the desired change that hetroepitaxy produces in the value of the poten-
tial.

The energy behavior at each surface site is monitored over a sampling
interval Δt_s, every sampling interval. The simulation of thermal energy
fluctuations is done by random number generation. For each site (i,j) we
generate a random energy $E(R)$ and add it to the interaction potential
$U_o(i,j)$ to obtain a total energy of

$$U(i,j) = U_o(i,j) + E(R). \tag{1}$$

This energy is then compared to energy barriers for desorption, surface
migration and incorporation. If the total energy exceeds one of these bar-
riers, we allow the adatom to proceed accordingly. If the total energy is
less than the lowest barrier, then the adatom remains localized. In sum-
mary, our Monte Carlo procedure entails the generation of a random energy
for each site and calculating a total energy U, if this value U is such
that:

      (a) $U < U_m$, the adatom remains localized;

      (b) $U_m < U < U_i$, surface migration is allowed to occur;

      (c) $U_i < U < U_e$, surface migration or incorporation into the
                     bulk is allowed to occur;

      (d) $U_e < U$, evaporation occurs.

During each time interval Δt_s, a random energy $E(R)$ was assigned to each of the surface adatoms. We let

$$U(i,j) = U_o(i,j) + E(R) \qquad (2)$$

denote the total energy possessed by a surface adatom at a site (i,j) during this time interval. This total energy is the sum of the potential energy U_o due to the lattice structure and a random energy E from a modified Boltzmann distribution to be discussed in the next section which characterizes the random surface energy. When U was less than some material-dependent migration level U_m, the adatom remained stationary at the surface site. If $U_m < U < U_e$, surface migration by random walk was allowed to occur. If U was greater than the evaporation potential U_e, the adatom was removed from the site and for $U_i < U < U_e$ incorporation or migration was assumed to occur.

The rate of impingement of adatoms upon the surface was independent of the surface configuration. The rates associated with the evaporation and migration of adatoms depended upon the potential barriers U_e and U_m and also upon the values assigned to the potential changes Φ_o and $-w_i$, ($i = 1, \ldots, 8$). These later potential changes had to take into account the type of crystal structure and orientation of the growth we were trying to simulate with the SOS model. In figure 5(a), for growth on the (100) face, we set up a correspondence between the central site, the nearest neighbor potentials ϕ_1, second nearest neighbor potentials ϕ_2, and the adatom potential changes for the mask in Table 1 (e.g., $w_1 = \phi_2$, $w_2 = \phi_1$). In a similar manner we were able to set up the correspondences illustrated in figure 5(b) and (c) for the (111) and (110) orientations. In Table 2, we selected the relation between the neighbor potentials $\phi_0, \phi_1, \phi_2, \phi_3$ in such a way that when the first level of adatoms covered the surface, the potential distribution returned to its original value. This produced the constraint conditions on the neighboring potentials which are illustrated in Table 2. We assumed that $\Phi_o = \Delta H_{ads}$ and were left with decisions on how to assign the ϕ_1, ϕ_2, ϕ_3 values. For the (100) orientation we let $\phi_3 = 0$ and were left with having to assign values to ϕ_1, ϕ_2. One possible choice was to assign ϕ_1 a value based upon nearest neighbor bond strength and then calculate the $\phi 2$ value based upon the constraint.

Alternatively, we let ϕ_1 denote the change in the nearest neighbor potentials due to the addition of an adatom to the surface and let ϕ_2, ϕ_3 denote the second and third nearest neighbor potential changes. We assumed that $\phi_2 = \alpha_2 \phi_1$ and $\phi_3 = \alpha_3 \phi_1$ where α_2, α_3 are scale factors which are less than one. This allowed us to define the crystal orientation factor ξ as

$$\xi = \begin{cases} 2 + 2\alpha_2 & , \quad (100) \\ 3 + 3\alpha_2 & , \quad (111) \\ 1 + \alpha_2 + 2\alpha_3, & (110) \end{cases} \tag{3}$$

which takes into account the different crystal orientations. We also defined the kink site potentials before $U_{ks}^{(1)}$ and after $U_{ks}^{(2)}$ and the capture of an adatom as $U_{ks}^{(1)} = U_0 - \xi\phi_1$, $U_{ks}^{(2)} = U_0 + \xi\phi_1$. (Note that $\Phi_0 = 2\xi\phi_1$.) Note that the values assigned to the mask potential changes are not necessarily the same for the different orientations: for example, the ϕ_1, ϕ_2, ϕ_3 values for each case in Table 2 could have different values.

We can assign arbitrary values to the neighbor potential changes ϕ_1, ϕ_2, ϕ_3 as long as these values satisfy the constraint that $\phi_0 = 2\xi\phi_1$. If we arbitrarily assign values to α_2, α_3 than we can solve for ϕ_1 and consequently ϕ_2, and ϕ_3. Instead of arbitrarily assigning values to α_2 and α_3, we examine a (m_0, n_0) Mie potential curve with $m_0 < n_0$ (ref. 15)

$$\phi = \phi^* \left[\left(\frac{R^*}{R} \right)^{n_0} - \frac{n_0}{m_0} \left(\frac{R^*}{R} \right)^{m_0} \right] \tag{4}$$

Here R^* is the distance at which ϕ obtains its minimum value of $\phi^* \left(1 - \frac{n_0}{m_0} \right)$. If we examine the potential values at various distances $R = a_0, \frac{\sqrt{2}}{2} a_0, \frac{\sqrt{3}}{2} a_0, \frac{\sqrt{3}}{2} a_0$, with $R^* = a_0$, then the ratio of the Mie potential values at these distances can be used to approximate the values of $\alpha_2 = \phi_2/\phi_1$ and $\alpha_3 = \phi_3/\phi_1$ for different crystal orientations and different m_0, n_0 values.

Table 2. Potential changes for addition of an adatom to an arbitrary site.

Crystal Face	Relation Between Neighbor Potentials	Potential Changes for Addition to Arbitrary Site	Distances to Neighboring Sites
		$$\begin{bmatrix} -\omega_7 & -\omega_8 & -\omega_1 \\ -\omega_6 & \phi_0 & -\omega_2 \\ -\omega_5 & -\omega_4 & -\omega_3 \end{bmatrix}$$	
(100)	$\phi_0 = 4\phi_1 + 4\phi_2$	$$\begin{bmatrix} -\phi_2 & -\phi_1 & -\phi_2 \\ -\phi_1 & -\phi_0 & -\phi_1 \\ -\phi_2 & -\phi_1 & -\phi_2 \end{bmatrix}$$	a_0, $\dfrac{\sqrt{2}}{2}a_0$
(111)	$\phi_0 = 6\phi_1 + 6\phi_2$	$$\begin{bmatrix} & -\phi_2 & & \\ -\phi_2 & -\phi_1 & -\phi_1 & -\phi_2 \\ & -\phi_1 & \phi_0 & -\phi_1 \\ -\phi_2 & -\phi_1 & -\phi_1 & -\phi_2 \\ & & -\phi_2 & \end{bmatrix} -\phi_2$$	$\sqrt{\dfrac{3}{2}}\,a_0$, $\dfrac{\sqrt{2}}{2}a_0$, $\dfrac{\sqrt{2}}{2}a_0$
(110)	$\phi_0 = 2\phi_1 + 2\phi_2 + 4\phi_3$	$$\begin{bmatrix} -\phi_3 & -\phi_2 & -\phi_3 \\ -\phi_1 & \phi_0 & -\phi_1 \\ -\phi_3 & -\phi_2 & -\phi_3 \end{bmatrix}$$	a_0, $\sqrt{\dfrac{3}{2}}a_0$, $\dfrac{\sqrt{2}}{2}a_0$
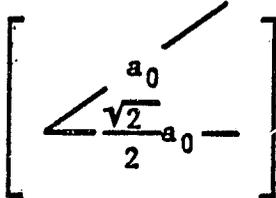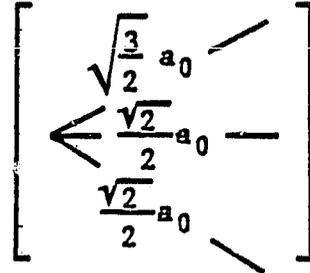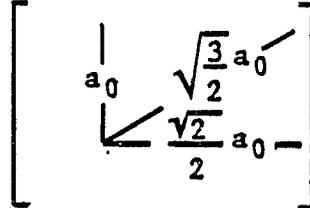
Energy Distribution and Time

During each sample interval Δt_s, an atom in an arbitrary site (i,j) has the total energy

$$U(i,j) = U_0(i,j) + E(R)$$

where $E(R)$ is determined by random number R from the Boltzmann distribution

$$f(E) = \lambda \exp[-\lambda E], \quad E > 0 \tag{5}$$

where $\lambda = 1/KT$ is the parameter of this exponential distribution. The mean energy of this distribution is

$$\langle E \rangle = \int_0^\infty E \, f(E) \, de = KT = \frac{1}{\lambda} \tag{6}$$

and the cumulative energy distribution is given by

$$F(E) = \int_0^E f(E) dE = 1 - \exp[-\lambda E]. \tag{7}$$

A random variate E can be generated from this distribution by using the inverse function associated with the cumulative distribution. For R a uniform random number between 0 and 1 and with $R = F(E)$, the inverse function gives the random energy

$$E = E(R) = -KT \ln(1 - R) \tag{8}$$

so that (1) becomes

$$U(i,j) - U_0(i,j) - KT \ln(1 - R) \tag{9}$$

The residence or stay-time of an adatom on a surface is given by the Frenkel equation (ref. 16)

$$\tau = \tau_0 \exp[-\lambda \, \Delta Hads] \tag{10}$$

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where ΔH_{ads} is the heat of adsorption and τ_0 is the period of vibration for the surface adatoms ($\tau_0 \sim 10^{-12}$ sec). Ideally then, the most physically real sampling time corresponding to changes in vibrational energy and, therefore, changes in $U(i,j)$ is to choose $\Delta t_s = \tau_0$. Computer costs and time, of course, prohibit the extensive amount of computations that would be necessary to sample 400 sites 10^{12} times each second. In order to circumvent this difficulty, the method of ordered statistics is applied. Essentially, most of the time-dependent energy variation at a particular site results in insufficient thermal energy for adatom movement and adatoms remain localized over most of the sampling interval. Since this large time of atomic localization is not important to the actual thin film growth, only the fraction of the sampling interval that movement does occur need be considered. Thus we desire that fraction of the time that the site energy is in excess of the minimum activation barrier for adatom activity.

Let E_1, E_2,...E_n denote n random samples from the exponential distribution (3) and let $E_{(1)}$, $E_{(2)}$,..., $E_{(\bar{n})}$ denote the ordered arrangement (from low to high) of the n random samples with $E_{(i-1)} < E_{(i)}$ for all $i=2,3,...,n$. The probability distribution of the largest ordered statistic $E_{(n)} = \max \{E_1, E_2,..., E_n\}$ is given by (ref. 17)

$$g(E) = n[F(E)]^{n-1} f(E), \quad 0 < E < \infty \tag{11}$$

where $f(E)$ and $F(E)$ are given by equations (3) and (5). The cumulative frequency distribution is given by

$$G(E) = \int_0^E g(E)dE = \left(1 - e^{-\lambda E}\right)^n \tag{12}$$

To generate a random variable $E_{(n)}$ from this distribution, a uniform random number R, with $0 < R < 1$, is generated such that $G\left(E_{(n)}\right) = R$, then the inverse function gives the random energy

$$E_{(n)} = - KT \ln \left(1 - R^{1/n}\right) \tag{13}$$

which can be compared with equation (6). Note that for large values of n, we can approximate the random energy $E_{(n)}$ by

$$E_{(n)} = - KT \, \ell n \left(- \frac{1}{n} \, \ell n \, R \right). \tag{14}$$

If for example, T = 500 K and the activation energy for diffusion is Q_d = 0.7 eV, then the mean time between hops is τ_d = 10^{-12} exp $[\lambda Q_d]$ = 10^{-5} sec or, in a sampling interval of Δt_s = 10^{-5} sec, a single hop occurs. Any smaller sampling interval is not necessary because no movement occurs. Any larger sampling interval would result in multiple events for a single adatom and the less physical the model becomes. Figure 6 illustrates the probability distribution of the ordered statistic $E_{(n)}$ with n = 10^7, 10^8, 10^9 at T = 500 K.

The minimum activation energy for diffusion (ref. 18) determines the sampling interval and therefore the number of random samples, n. We make the following assumptions concerning the activation barriers for adatom activity (see figure 3): U_o = $\Delta Hsub$, U_e = 0, ϕ_o = $\Delta Hsub$ - $\Delta Hads$, U_m = $-\Delta Hads$ + Q_d, τ_d = τ_o exp (λQ_d), then the mean number of hops in Δt_s sec is given by $\Delta t_s / \tau$ and n = $\Delta t_s / \tau_o$. Let Δt_o denote the output "snapshot" time interval where we perform a stop action and view the surface. The number of surface scans during this time interval is given by $\Delta t_o / \Delta t_s$. For example, if Δt_o = 0.1 and Δt_s = 10^{-4} we would scan each of the 400 surface sites 10^3 times and generate $4(10^5)$ random energies $E_{(n)}$ from the modified Boltzmann ordered statistic probability distribution.

Random Walk and Incorporation

For a fixed uniform deposition rate R_d, adatoms are deposited at random positions on the surface based upon the value assigned to Δt_s. For small Δt_s, we must wait for some multiple of this time before adding a single adatom. Each time an adatom is deposited, or removed from a site, the potentials surrounding the site are updated. In the case of surface migration, an adatom has sufficient energy to migrate and we treat migration as an evaporation followed by a deposition at a neighboring site. The availability of more than one site for migration is another decision which is made according to the ligancy or coordination number associated with the

available sites. From an interaction potential perspective, this is physically reasonable since the site that has a deeper well (more attractive) will have an energy barrier to migration that is smaller, thus having a higher probability for migration to that site. The experimental evidence to support this assumed behavior is sizeable (ref. 19). Each unoccupied nearest neighbor and second neighbor site is given a weight which is the ligancy if an adatom had random walked to that site. These weights are then normalized and a weighted random walk to one of these sites is determined by a random number. If all nearest neighbor and second nearest neighbor sites are occupied, the adatom is assumed to jump up onto the next level at an unoccupied nearest neighbor site with equal probability.

In the case $U_i < U < U_e$, an adatom is considered to be either incorporated or to surface migrate by weighting the two possibilities according to their relative probabilities. In the case of incorporation an adatom is removed from the surface in the same way an adatom desorbs. It is assumed that the bulk vacancy concentration is sufficient to receive the adatoms and therefore the adatom just disappears from the surface site. The excess energy after an event is assumed to be reabsorbed into the thermal energy of the solid.

Generalizations

Various modifications and extensions of the ideas presented in the previous sections will make the model more general. Some of the modifications will be presented in this section as these reflect modifications of the SOS model. Three-dimensional model concepts which differ from the SOS model concepts will be presented in a later section.

As adatoms are deposited upon the surface we will label them as "A-type" or "B-type" where the A-types represent substrate adatoms and the B-types represent the growing material. As the vertical growth increases the fraction of A's mixed with the B's is allowed to decrease. In this way we can simulate adatom diffusion through the growing film to the surface by randomly depositing substrate adatoms on the surface, at a rate controlled by the diffusions equations for the adsorbate/adsorbent system. Also,

instead of one potential change mask we will introduce four such masks to reflect the potential changes associated with the deposition process of: A on A, A on B, B on A, or B on B type of interactions. This additional complexity increases the bookkeeping to keep track of where the A and B type adatoms are located.

By judicially choosing the A on A, A on B, B on A, and B on B potential changes we can use the SOS model to simulate A-B type crystal growth. By assigning an initial substrate of an A-B checkerboard pattern we can make the A on A interaction subject to a high probability of migration of A adatoms to a nearest neighbor B-site. Similar considerations hold for B on B interactions. The nature of interatomic potentials (ref. 20) can also be varied from site to site.

Description of the Computer Program

A flowchart of the computer program is given in figure 7 and the FORTRAN computer program is presented in Appendix A. The program is liberally spiced with comment statements to help the reader. An attempt was made to make the program modular in character in the event extensive revision was needed. The following is a brief description of the subroutines:

Program Crystal

Here parameters are read in and other variables are initialized and, before the program actually runs, a printout of all initial values and parameters is made.

Subroutine SETUP

Assumes a (m_o, n_o) Mie potential and calculates ϕ_1, α_2, α_3 given the initial value for ϕ_0.

Subroutine FACE

Calculates the potential changes associated with a (100), (111), or (110) crystal orientation and distances to nearest neighbor site.

Subroutine INITIAL

Initializes and prints out the substrate geometry and assigned values of the potentials at each site.

Subroutine DIFF

A weighted random walk surface diffusion is simulated by an evaporation followed by a deposition at the nearest neighbor site.

Subroutine PBOND

Calculates the weights associated with the random walk processes on one of the crystal orientations.

Subroutine ADATOM

Updates the potential sites at i,j and the surrounding neighbor sites when an adatom is added to site (i,j).

Subroutine SUBATOM

Updates all neighboring potentials when an adatom is removed from a site (i,j).

Subroutines EDGE, EDD, XYX, CORRECT

The geometry of the 20×20 square array assumes periodic boundary conditions as illustrated in figure 8. This 20×20 array is embedded into a 24×24 square array and addition or removal of adatoms along an edge, or migration across an edge, requires that the outer border of the 24×24 array be updated to reflect the periodic conditions. These periodic conditions are maintained by the subroutines EDGE, EDD, XYX. and CORRECT.

Subroutine STOFIN

Starts and finishes a computer run. This subroutine analyzes the deposition rate and scan time and deposits adatoms on the surface, if required. Surface scanning of each site is performed and computer output is printed.

Subroutine URNS

Calculates random sites and type of adatom (A or B) to be deposited on the surface.

Subroutine UPDATE

Scans the top layer of the surface and counts the size and frequency of clusters. Also calculated are coverage for the two highest layers, roughness factor, and number of A and B type adatoms on the surface.

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Subroutine MIXUP

Takes the vector $(1,2,3,\ldots,N)$ and randomizes the position of the integers to form a vector $(u_1,u_2,u_3,\ldots,u_N)$ which is some rearrangement of the initial vector.

Subroutine GROW

Optional computer graphics of output data.

COMPUTER RESULTS AND DISCUSSIONS

Various computer experiments were performed with the model. These experiments are listed in Table 3. The computer experiments were performed for a (100) fcc surface to assess the physical behavior of the model.

Because there exists no real data on semiconductor crystals for the interaction and potential energy changes associated with adatom movement, we chose the following set of nominal parameters:

ΔHads = 1.7 eV

ΔHsub = 3.87 eV

D_{-z} (Ge/Ge) = 7.8 exp $(-2.98\ \lambda)$ cm^2 s^{-1}

D_{-z} (Si/Fe) = 0.44 exp $(-2.09\ \lambda)$ cm^2 s^{-1}

D_{+z} (Fe/Ge) = 0.13 exp $(1.08\ \lambda)$ cm^2 s^{-1}

Q_d = 0.7 eV

$S = S_i = 1$

which represents the best available data for a Germanium type system.

In experiment 1, we examined the surface migration of a single adatom which performed a random walk to the nearest neighbor sites whenever the random energy associated with a single scan dictated such behavior. The number of migrations as a function of time is linear and varies exponentially with temperature. Figure 9 shows a plot of diffusion coefficient vs.

Table 3. Computer experiments.

Experiment	Deposition Rate $(cm^{-2}s^{-1} \times 10^{15})$	Temperature (K)	Run Time
1. Surface diffusion of a single adatom	0	400, 500, 600	2
2(a) Nine adatoms in a row	0	400, 500, 600	2
(b) Nine adatoms randomly distributed	0	400, 500, 600	2
3. Thin film growth with defect site	0.5	400, 500, 600	2
4. Thin film growth with variable deposition rate	0.25, 0.5, 1, [2.5 (10^{-3})]	500 400	2 40
5. Thin film growth with variable substrate temperature	0.5, 1.0	300, 400, 500 600, 700	2
6. Annealing of thin film growth	0	600, 700	6

inverse temperature as calculated from the computer model. The linear be-
havior of the diffusion constant follows from the equation

$$D = \frac{\ell \, a_o^2}{\tau_o} \exp \, (-\lambda Q_d) \tag{15}$$

where a_o is the jump distance and $\ell = 1/4$ for a (100) face. The slope
of the Arrhenius plot yields the activation barrier $Q_d = 0.7$ eV which is
our input condition. This provides a self consistent check on the physics
of the computer model. In figure 9, the number by the circles is the
average number of migrations for each temperature given. The results in
experiment 1 are for a flat surface. In the case of nonuniform surface the
mean diffusion length and migration frequency would be substantially reduced
due to the lower probability of escape from kink sites, steps and other
defects.

In experiments 2(a,b) we examined the clustering of lineal and randomly
dispersed adatoms as a function of temperature. In both cases the adatoms
tended to seek out the most stable configuration in that each adatom ulti-
mately tried to maximize its number of nearest neighbors and hence form a 3
× 3 array. In the first case 2(a) the lineal adatoms were all connected and
the probability of adatoms breaking away from the row increased with temper-
ature. The adatoms tended to form stable clusters with the migration of
single adatoms along a step being the dominant form of motion. For this
experiment a 3 × 3 array was the most stable cluster. In the second case
2(b) the dispersed adatoms performed random walks and collided to form
dimers, trimers, and eventually a nine adatom cluster. Figure 10 is a
graphic display of the sequence of events as a function of time. At some of
the temperatures the 3 × 3 array was not completely achieved. However,
given sufficient time, these configurations eventually became a 3 × 3 array.

The question of cluster growth is perceived to occur by either adatom
capture or by actual enmasse motion of one of the smaller clusters into a
larger cluster. The subsequent collision and reorientation of the adatoms
to registry with the second cluster was assumed to occur. In the formula-
tion of this model no consideration was given to the motion of whole

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clusters, but as these computer experiments show whole clusters can move by individual adatom motion at the periphery of the cluster resulting in a net motion of its center of mass [see figures 10(b,c)].

In experiment 3, a generalized point defect was modeled by adjusting the potential to be very large at a single point and its four nearest neighbors sites. After one layer covered this site only the central site was allowed to have a larger potential and after a second layer the potential was allowed to return to the normal value of that of its neighbors. Figure 11 shows the prescribed potential changes for the first two layers of growth. After the second layer covered the trap, the potential was allowed to return to its normal value. Figure 12 illustrates the effect of a trap and the resulting growth around the trap for a constant deposition rate and several surface temperatures. Many interesting phenomena occurred in our study of a trap and we will pursue this case in more detail in a later report. For the time being, a brief description of the observed phenomena will have to suffice. At low temperatures the surface adatoms initially adsorbed do not statistically interact with the site and ordinary homogeneous nucleation and growth occurs uniformly over the surface. As adatoms impinge upon the trap site heterogeneous nucleation occurs and growth is much more rapid in this vicinity. Further the vertical growth in the vicinity of the trap is initially larger because the potential at the trap site is still lower after being covered by the first layer which is an island upon which impinging adatoms can migrate and find this lower potential. It is thus likely that the growth in the vicinity of the trap would be dominated by this effect. At higher temperatures the major growth occurs by way of vapor phase transport as opposed to surface defect density (ref. 21) and to the magnitude of the deposition rate. Growths have been achieved at very low temperatures on appropriate substrates if, and only if, the surface was relatively smooth and defect free as determined by Kikuchi lines present in the RHEED patterns. If the defect density is too high, then epitaxy is inhibited by the dominance of growth from the defects. If the deposition rate is too high then even with low defect density the growth around a defect is so rapid that epitaxy is also limited. Therefore, the understanding of the growth rate about different types of defects would be helpful in assessing the probability of epitaxy for a given system, and we will pursue these questions at a later time.

In experiment 4, we varied the deposition rate (1 nm/sec = 1.8 (10^{15}) adatoms/cm^2 sec), and figure 13 illustrates the effect of this variation on the surface roughness. More experimentation in this area is necessary as we will see from the next computer experiment, which also includes variable deposition rates.

In experiment 5, the substrate temperature was varied. Figures 14-17 illustrate the effect of this variation. The uniformity of the surface is progressively improved as the temperature increases and the deposition rate decreases. Figure 13 illustrates the roughness factor as a function of time and demonstrates the changing surface uniformity. The oscillatory nature of the curves is a consequence of the growing multilayers and that surface migration tends to fill in the vacancies, ledges and kink sites. The surface adatoms becomes more mobile at the higher temperatures and tend to fill in these sites. This behavior has been observed by Weeks and Gilmer (ref. 6) for crystal growth from the melt. Figures 14(a-c) illustrate the growth sequence at T = 300 K as compared to figures 14(d-f) which show the growth sequence at T = 400 K. Figure 15 illustrates the growth sequence for R_d = 0.2778 nm/sec and T = 500 K. Figure 16 illustrates growth occurring by an advancing ledge that was formed upon the coalescence of two large clusters. Growth by this mechanism has been discussed by Weeks and Gilmer (ref. 6), but in this particular case it is statistical in nature rather than the dominant phenomena.

Coalescing clusters at submonolayer levels have been illustrated in figure 15 to show the possible development of a grain boundary. Although a graphic representation of different growing grain orientations is not easily done with the SOS model, the potential field surrounding a particular defect or nucleation site does provide some information on the probable growth orientation and, therefore, may permit a way of deciding if the coalescing grains will be in, registry, near registry (low angle grain boundary) or whether a high angle grain boundary will be formed.

A plot of nucleation density n_s and maximum cluster size N_s as a function of time is given in figure 19 for a deposition rate of 0.2778 nm/sec. Clusters of size n_i (i > 1) have a total density of

$$\sum_{i=z}^{\infty} n_i = n_s .$$ (16)

Definite maxima are observed for all temperatures tested. As is apparent from the time frames of figures 14-17, the decay in n_8 is due to the growth coalescence of clusters. This behavior has also been observed by Donahoe and Robbins (Au/NaCl) (ref. 22), Hamilton and Logel (Ag/C,Pd/C) (ref. 23), and Corbett and Boswell (Ag/MoS$_2$) (ref. 24). The maximum cluster size is also shown to decrease with increasing temperature as was also observed by Poppa for (Bi/C,Ag/C) (ref. 25). The most probable size of clusters for the maxima at T = 300 K and t = 5.5 sec. is approximately 2-3 adatoms. The initial slope of these curves is the nucleation rate which is given by

$$
T_o = z\sigma^* \ \frac{R}{\nu_o} \ ^{i^*+1} \exp \left[\frac{E_i^* + (i^*+1) \ \Delta Hads - Q_d}{KT} \right]
\tag{17}
$$

where z is the Zeldovitch factor, σ^* is the capture number, E_i^* is the cluster energy, and i^* is the critical cluster size.

In experiment 6, we studied the effects of annealing. In a similar manner to the ordering that occurs in experiment 2, the annealing of a given deposition of growth proceeds by surface diffusion or monologue exchange between clusters (Ostwald ripening). As discussed previously, cluster peripheral motion may also occur to effect an increase in the order of the growth. Figure 20(a) illustrates the initial growth condition used in our study. Then with R_d = 0, the substrate temperature is increased. Each island or cluster is driven to maximize its number of nearest neighbors giving rise to more ordered arrangements as shown in figures for the anneal temperatures of T = 600 and t = 700 K. Note that the number of smaller nuclei has not noticeably decreased. Figure 19 shows the effect of temperature on the average density of the clusters. This same sort of behavior was observed by Donohoe and Robins for the Au/NaCl system. Annealing at deposition temperature did not seem to have a significant effect even for large times. However, when the temperature was increased the low density clusters ultimately broke up by nonomer exchange to the larger more stable clusters.

In the (1ī1) face we assumed that ϕ_2 = 0 for ease of computation and results for the other crystal faces (111) and (11υ) are not yet available at this time.

THREE-DIMENSIONAL CONCEPTS AND EXTENSIONS OF MODEL

In order to get away from a SOS model one must get involved with the three-dimensional geometry of crystal growth. With this purpose in mind, consider figure 21 which illustrates a set of orthogonal axes with basis vectors $\vec{e}_1 = \frac{a_o}{2}\hat{i}$, $\vec{e}_2 = \frac{a_o}{2}\hat{j}$, $\vec{e}_3 = \frac{a_o}{2}k$ together with a cubic (P), body centered (I) and face centered (F) lattices.

For the simple cubic lattice all crystal lattice sites are given by

$$\vec{r} \simeq 2\ell\,\vec{e}_1 + 2m\vec{e}_2 + 2n\vec{e}_3$$

where ℓ, m, n are integers. From any lattice point there are six nearest neighbor (NN) positions given by the directions $\pm\,(\vec{n}_1,\ \vec{n}_2,\ \vec{n}_3)$ where $\vec{n}_1 = 2\vec{e}_1$, $n_2 = 2\vec{e}_2$, $\vec{n}_3 = 2\vec{e}_3$. There are 12 second nearest neighbors (SNN) given by the directions $\pm\,(\vec{s}_1,\ \vec{s}_2,\ \vec{s}_3,\ \vec{s}_4,\ \vec{s}_5,\ \vec{s}_6)$ where $\vec{s}_1 = \vec{n}_1 + \vec{n}_2$, $\vec{s}_2 = \vec{n}_2 + \vec{n}_3$, $\vec{s}_3 = \vec{n}_1 + \vec{n}_3$, $\vec{s}_4 = \vec{n}_1 - \vec{n}_3$, $\vec{s}_5 = \vec{n}_2 - \vec{n}_3$, $\vec{s}_6 = \vec{n}_1 - \vec{n}_2$. There are 8 third nearest neighbors (TNN) given by $\pm\,(\vec{t}_1,\ \vec{t}_2,\ \vec{t}_3,\ \vec{t}_4)$ where $\vec{t}_1 = \vec{n}_1 + \vec{n}_2 + \vec{n}_3$, $\vec{t}_2 = \vec{n}_1 - \vec{n}_2 + \vec{n}_3$, $\vec{t}_3 = \vec{n}_1 + \vec{n}_2 - \vec{n}_3$, $\vec{t}_4 = \vec{n}_1 - \vec{n}_2 - \vec{n}_3$.

For the body centered cubic lattice, all sites are given by

$$\vec{r} = 2\ell\,\vec{e}_1 + 2m\vec{e}_2 + 2n\vec{e}_3, \qquad \ell, m, n \text{ integers}$$

together with the set of points

$$\vec{r} = (2I+1)\vec{e}_1 + (2J+1)\vec{e}_2 + (2K+1)\vec{e}_3, \qquad I, J, K \text{ integers.}$$

For the neighboring atoms about a given point we have the following directions:

NN directions (8 total) $\pm\,(\vec{n}_1,\ \vec{n}_2,\ \vec{n}_3,\ \vec{n}_4)$

$$\vec{n}_1 = \vec{e}_1 + \vec{e}_2 + \vec{e}_3, \quad \vec{n}_2 = \vec{e}_1 + \vec{e}_2 - \vec{e}_3, \quad \vec{n}_3 = \vec{e}_1 - \vec{e}_2 + \vec{e}_3$$

$$\vec{n}_4 = \vec{e}_1 - \vec{e}_2 - \vec{e}_3$$

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SNN directions (6 total) $\pm (\vec{s_1}, \vec{s_2}, \vec{s_3})$

$$\vec{s_1} = 2\vec{e_1}, \quad \vec{s_2} = 2\vec{e_2}, \quad \vec{s_3} = 2\vec{e_3}$$

TNN directions (12 total) $\pm (\vec{t_1}, \vec{t_2}, \vec{t_3}, \vec{t_4}, \vec{t_5}, \vec{t_6})$

$$\vec{t_1} = \vec{s_1} + \vec{s_2} \qquad \vec{t_4} = \vec{s_2} - \vec{s_3}$$

$$\vec{t_2} = \vec{s_1} + \vec{s_3} \qquad \vec{t_5} = \vec{s_1} - \vec{s_3}$$

$$\vec{t_3} = \vec{s_2} + \vec{s_3} \qquad \vec{t_6} = \vec{s_1} - \vec{s_2}$$

Similarly, we find for the face centered cubic crystal that all lattice sites are given by

$$\vec{r} = 2\ell \vec{e_1} + 2m\vec{e_2} + 2n\vec{e_3}, \qquad \ell, m, n \text{ integers}$$

together with the set of points

$$\left. \begin{aligned} \vec{r} &= (2I+1)\vec{e_1} + (2J+1)\vec{e_2} + 2K\vec{e_3} \\ \vec{r} &= 2I \vec{e_1} + (2J+1)\vec{e_2} + (2K+1)\vec{e_3} \\ \vec{r} &= (2I+1)\vec{e_1} + 2J\vec{e_2} + (2K+1)\vec{e_3} \end{aligned} \right\} \quad I, J, K \text{ integers}$$

For the neighboring adatoms we have:

NN directions (12 total) $\pm (\vec{n_1}, \vec{n_2}, \vec{n_3}, \vec{n_4}, \vec{n_5}, \vec{n_6})$

$$\vec{n_1} = \vec{e_1} + \vec{e_2} \qquad \vec{n_4} = \vec{e_1} - \vec{e_3}$$

$$\vec{n_2} = \vec{e_2} + \vec{e_3} \qquad \vec{n_5} = \vec{e_2} - \vec{e_3}$$

$$\vec{n_3} = \vec{e_1} + \vec{e_3} \qquad \vec{n_6} = \vec{e_2} - \vec{e_1}$$

SNN directions (6 total) $\pm (\vec{s_1}, \vec{s_2}, \vec{s_3})$

$$\vec{s_1} = 2\vec{e_1}, \qquad \vec{s_2} = 2\vec{e_2}, \qquad s_3 = 2\vec{e_3}$$

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TNN directions (24 total) $\pm (\vec{t_1}, \vec{t_2}, \vec{t_3}, \vec{t_4}, \ldots, \vec{t_{12}})$

$$\vec{t_1} = 2\vec{e_1} + \vec{e_2} + \vec{e_3}$$

$$\vec{t_2} = 2\vec{e_1} + \vec{e_2} - \vec{e_3}$$

$$\vec{t_3} = \vec{e_1} + 2\vec{e_2} + \vec{e_3}$$

$$\vec{t_4} = \vec{e_1} + 2\vec{e_2} + \vec{e_3}$$

$$\vec{t_5} = \vec{e_1} + \vec{e_2} + 2\vec{e_3}$$

$$\vec{t_6} = \vec{e_1} + \vec{e_2} - 2\vec{e_3}$$

$$\vec{t_7} = -2\vec{e_1} + \vec{e_2} + \vec{e_3}$$

$$\vec{t_8} = -2\vec{e_1} + \vec{e_2} - \vec{e_3}$$

$$\vec{t_9} = -\vec{e_1} + 2\vec{e_2} + \vec{e_3}$$

$$\vec{t_{10}} = -\vec{e_1} + 2\vec{e_2} - \vec{e_3}$$

$$\vec{t_{11}} = -\vec{e_1} + \vec{e_2} + 2\vec{e_3}$$

$$\vec{t_{12}} = -\vec{e_1} + \vec{e_2} - 2\vec{e_3}$$

For a three-dimensional model of crystal growth we imagine an infinite number of lattice sites of one of the three types discussed. We assign some initial geometry of occupied sites in the first octant and assume symmetry conditions at the boundaries which separate the first octants from the other (in order to simplify the upcoming bookkeeping). Each occupied site has a potential determined by the number of NN, SNN, and TNN sites which are occupied and we write

$$U(i,j,k) = NN_{ijk}\, \phi_1 + SNN_{ijk}\, \phi_2 + TNN_{ijk}\, \phi_3$$

Note that the maximum potential when all bonds are in effect are given by:

$$\text{SC:} \quad U = 6\phi_1 + 12\phi_2 + 8\phi_3$$

$$\text{BCC:} \quad U = 8\phi_1 + 6\phi_2 + 12\phi_3 \tag{18}$$

$$\text{FCC:} \quad U = 12\phi_1 + 6\phi_2 + 24\phi_3$$

Here (ϕ_1) SC does not equal (ϕ_1) BCC which does not equal (ϕ_1) FCC. The symbol ϕ_1 is used to denote the nearest neighbor bond associated with a fixed crystal type. Similar considerations hold for the SNN and TNN bonds ϕ_2, ϕ_3.

Having defined an initial geometry we can label those occupied crystal sites, where the total bond structure is incomplete, as occupied surface sites (OSS). Those lattice sites which are unoccupied, and which are needed to complete the bonding of OSS, are labeled unoccupied surface sites (USS). Consider only those OSS and USS in the first octant. We can randomly deposit adatoms onto USS and convert these sites to OSS or bulk surface sites and simultaneously update the potentials at all NN, SNN, and TNN sites effected by the deposition as well as recording of the creation of any new USS. We can also scan all OSS and assign a random thermal energy to the potentials at these sites and determine whether the adatoms at these sites remain localized, migrate to NN or SNN sites, incorporate or evaporate. Again, the recording of all potential changes of the sites involved, as well as the updating of OSS and USS locations, must be performed.

In order to analyze the three-dimensional growth, the following is proposed: Consider the plans illustrated in figure 10 which have direction numbers $[h_1, h_2, h_3]$. This plane passes through the point (Ia, 0, 0) and can be expressed

$$h_1 x + h_2 y + h_3 z = Ih_1 a \tag{19}$$

where I is an fixed integer and h_1, h_2, h_3 are integers. We next construct the vectors $\vec{A}$, $\vec{B}$, $\vec{C}$ which also lie in the plane and are defined as

$$\vec{A} = -h_1 \vec{e_3} + h_3 \vec{e_1}$$
$$\vec{B} = -h_1 \vec{e_2} + h_2 \vec{e_1} \tag{20}$$
$$\vec{C} = h_2 \vec{e_3} - h_3 \vec{e_2}$$

Let $\vec{r_o} = 2I\vec{e_1}$ be a vector to (Ia, 0, 0). Then, to determine all lattice sites in this plane, we determine rational numbers f, g such that for a given crystal structure,

$$\vec{r} = \vec{r}_0 + f\vec{B} + g\vec{A} = x\vec{e}_1 + y\vec{e}_2 + z\vec{e}_3$$

where x, y, z are lattice sites. In the case of a simple cubic crystal we would require that

$$2I\vec{e}_1 + f(h_1\vec{e}_2 - h_2\vec{e}_1) + g(h_1\vec{e}_3 - h_3\vec{e}_1) = 2\ell\vec{e}_1 + 2m\vec{e}_2 + 2n\vec{e}_3$$

where I, h_1, h_2, h_3, ℓ, m, n are integers. This equation requires that

$$2I - fh_2 - gh_3 = 2\ell$$
$$fh_1 = 2m$$
$$gh_1 = 2n$$

For these equations to possess integer solutions, ℓ, m, n must satisfy

$$hI = h_1\ell + h_2m + h_3n \qquad (21)$$

Consider first the case $I = 0$, then integer solutions (ℓ, m, n) to $h_1\ell + h_2m + h_3n = 0$ are given by the points $A = (h_3, 0, \overline{h}_1)$, $B = (h_2, \overline{h}_1, 0)$ and $C = (0, h_3, \overline{h}_2)$. These points define the primitive vectors $\vec{A}$, $\vec{B}$, $\vec{C}$ in (20) and the primitive cells in figure 22. The primitive cell A, $\overline{B}$ has a maximum of (h_1-1) interior solutions. Similarly, the primitive cells $\overline{B}$, $\overline{C}$ and $\overline{A}$, $\overline{C}$ have a maximum of h_2-1 and h_3-1 solutions. In the primitive $\overline{A}$, $\overline{B}$ cell of figure 22, we let n take on the integer values from 1 to (h_1-1). For a fixed value of n we let m vary from $\overline{1}$ to $(\overline{h}_1-1)$ and find the integer solution for the other variable ℓ. A similar analysis applies to the primitive cells $\overline{B}$, $\overline{C}$ and $\overline{A}$, $\overline{C}$.

Example: Consider the (295) plane of a simple cubic crystal. Here we want integer solutions (ℓ, m, n) to the equation

$$2\ell + 9m + 5n = 0$$

We take the obvious solutions $(0, 0, 0)$, $A = (5, 0, \overline{2})$, $B = (9, \overline{2}, 0)$ and $C = (0, 5, \overline{9})$ and construct primitive cells. For the $\overline{A}$, $\overline{B}$ cell we let $n = \overline{1}$ and let $m = \overline{1}$ (only one solution) and solve for ℓ. Thus we develop for

$n = \bar{1}$ the equation, $2\ell + 9m - 5 = 0$ with the solution of $(7, \bar{1}, \bar{1})$. Other solutions are $(7 - 9K, \bar{1} - 2K, \bar{1})$. $K = \pm 0, 1, 2,...$ Similarly, for the $\overrightarrow{A}, \overrightarrow{C}$ primitive cell, we let $\ell = 1, 2, 3, 4$ and $m = 1, 2, 3, 4$ and we solve for n. Thus:

for $\ell = 1$, $2 + 9m + 5n = 0$ and for $m = 1, 2, 3, 4$ we find $(1, 2, \bar{4})$ is the solution with $(1, 2 + 5K, -4 - 9K)$ as the general solution;

for $\ell = 2$ $(4 + 9m + 5n = 0) \rightarrow (2, 4, \bar{8}) \rightarrow (2, 4 + 5K, -8 - 9K)$;

for $\ell = 3$, $6 + 9m + 5n = 0 \rightarrow (3, 1, \bar{3}) \rightarrow (3, 1 + 5K, \bar{3} - 9K)$;

for $\ell = 4$, $8 + 9m + 5n = 0 \rightarrow (4, 3, \bar{7}) \rightarrow (4, 3 + 5K, -7 - 9K)$;

For the $\overrightarrow{B}, \overrightarrow{C}$ primitive cell we let $n = \bar{1}, \bar{2}, \bar{3}, \bar{4}, \bar{5}, \bar{6}, \bar{7}, \bar{8}$ and $\ell = 1, 2, 3, 4, 5, 6, 7, 8$ and solve for integer solutions m. This gives

$$n = -1, \quad 2\ell + 9m - 5 = 0 \rightarrow (7, \bar{1}, \bar{1}) \rightarrow (7, + 9K, \bar{1} - 2K, \bar{1})$$

$$n = -2, \quad 2\ell + 9m - 10 = 0 \rightarrow (5, 0, \bar{2}) \rightarrow (5 + 9K, - 2K, \bar{2})$$

$$n = -3, \quad 2\ell + 9m - 15 = 0 \rightarrow (3, 1, \bar{3}) \rightarrow (3 + 9K, 1 - 2K, \bar{3})$$

$$n = -4, \quad 2\ell + 9m - 20 = 0 \rightarrow (1, 2, \bar{4}) \rightarrow (1 + 9K, 2 - 2K, \bar{4})$$

$$n = -5, \quad 2\ell + 9m - 25 = 0 \rightarrow (8, 1, \bar{5}) \rightarrow (8 + 9K, 1 - 2K, \bar{5})$$

$$n = -6, \quad 2\ell + 9m - 30 = 0 \rightarrow (6, 2, \bar{6}) \rightarrow (6 + 9K, 2 - 2K, \bar{6})$$

$$n = -7, \quad 2\ell + 9m - 35 = 0 \rightarrow (4, 3, \bar{7}) \rightarrow (4 + 9K, 3 - 2K, \bar{7})$$

$$n = -8, \quad 2\ell + 9m - 40 = 0 \rightarrow (2, 4, \bar{8}) \rightarrow (2 + 9K, 4 - 2K, \bar{8})$$

The example illustrates that we can determine and count the coverage of a given region in a given plane. A similar counting procedure can be established for all parallel regions in planes parallel to a given plane as in figures 10(b-c). We can then plot coverage vs. distance as we move outward on parallel planes. Eventually, the coverage becomes zero and we can stop our counting procedure. Those directions for which the coverage vs.

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distance curves are like step functions, can be labeled as preferred directions of growth. Also the distance in these directions (number of growth planes measured from some reference) will increase with time at a faster rate than other nonpreferred growth directions. During the simulation of a three-dimensional crystal growth only the lower ordered planes need to be considered as the majority of the growth occurs on these planes.

CONCLUSIONS

An SOS Monte Carlo computer simulation utilizing a potential scaling technique has been developed to model the initial stages of thin film growth. The model makes use of ordered statistics to simulate the surface activity of a 20 × 20 array with periodic boundary conditions. Adsorption, desorption, surface migration, incorporation and substrate atom diffusion to the surface are considered. The results of several computer experiments show consistency with the expected behavior of thin-film growth. Surface migration data taken at different substrate temperatures returned the activation energy as determined by an Arrhonius plot. Dispersed adatoms were observed to cluster into dimers, trimers, and finally a single cluster in its most stable configuration. A point defect was designed by varying the interaction potential in the x, y, z directions and illustrated that preferred growth occurred at such defects. This suggests a technique for studying such defects.

The experimentation, with varying deposition rate and substrate temperature, modeled the expected behavior of thin film growth by nucleation, cluster growth and then coalescence of clusters. The nucleation rate was proportional to the square of the deposition rate in agreement with the atomic theory of nucleation. Finally, annealing experiments showed the time ordering of clusters with increased temperatures.

By adjusting the potential interaction changes and by varying the initial geometry and type of surface adatoms, various A-B crystal growth models can be investigated. The choice of the A on B, A on A, B on B or B on A interaction should produce interesting types of thin film growth phenomenon, and this area still has to be investigated. Also three-dimensional extensions will require large computer times and storage, but the basic scanning, testing and updating of potentials will be the main concern.

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ACKNOWLEDGEMENTS

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APPENDIX: COMPUTER PROGRAM

The following computer program is representative of that used in the studies of this report. It evolved from earlier models and is currently undergoing changes in order to better simulate and model AB, AA, BA, and BB types of crystal growth. Graphics output is illustrated in figure 23.

```
      PROGRAM CRYSTAL(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT,SSET,
     1TAPE7=SSET)
      COMMON/BLK1/H,EPS(30,30),ITRAC(30,30,20)
      COMMON/BLK2/UO,UM,UE,UOS,UMS,UES,DELT
      COMMON/BLK3/XLAM,TSNAP,M,T,TMIG,IEVAP,ICREAT
      COMMON/BLK4/FAA(9),D(9),FAB(9),FBA(9),DS(9),FBB(9)
      COMMON/BLK5/LAYER(30,30)
      COMMON/BLK6/N1,N2,LETA,M2,LAST
      COMMON/BLK7/PHI1,PHI2,PHI3,PHIO,J,PHS1,PHS2,PHS3,PHSO
      COMMON/BLK8/ISWTCH
      COMMON/BLK9/A,AS,EVIB,EVIBS,RD
      COMMON/BLK10/LL1,LL2,U1,MAXH,TA,TB
      INTEGER H(30,30)
      NAMELIST/PARAM/M,J,T,DELT,MO,NO,MOS,NOS,PHIO,PHSO,
     1RD,TSNAP,ISWTCH,A,AS,TSTOP,UO,UM,UE,UOS,UMS,UES,U1
C     NAMELIST VARIABLES   M=20 IS SIZE OF ARRAY,J=1(100)SURFACE,J=2 (111)SUR
C     J=3 (110)SURFACE,T=TEMP DEG K,DELT=TIME INTERVAL OF SCAN,NO,MO MIE
C     POTENTIAL OF GROWING MATL,MOS,NOS,MIE POTENTIALSFOR SUBSTRATE
      M=20  $  J=1  $  T=500.  $  DELT=1.0E-4 $ MO=4 $NO=10
      MOS=4 $NOS=10 $ PHIO=2.17 $PHSO=2.17 $TREF=300.$TSTOP=2.
      RD=200. $ TSNAP=.1 $UO=-3.87 $ UOS=-3.87 $ UM=-1.
      UMS=-1. $UE=0. $ UES=0. $ U1=1.7 $ A=5.61 $ AS=3.7
      ISWTCH=0
C     ISWTCH=1 GIVES PICTURES, ISWTCH=0 NO PICTURES IF ISWTCH=0
C     SET R1=0 IN JCL AND IF ISWTCH=1,SET R1=0 IN JCL(AFTER LGO)
C     INTERACTION WITH SUBSTRATE,PHIO=HEAT EVAP-HEAT ADSORPTION, PHSO IS PHIO
C     OF SUBSTRATE SURFACE,&0=RATE OF ADATOM DEPOSIT,ADATOMS/SEC,
C      A,AS,CRYSTAL LATTICE SPACING,TSTOP=STOP TIME,UO=HEAT EVAP,UM=
C     MIGRATION BARRIER,ASSUMED CONSTANT,UE=OIS EVAP REFERENCE,U1 NOT USED NOW
C     POTENTIAL ENERGIES IN ELECT. VOLTS U EV=23KCAL/MOLE,M=20 FOR GRAPHICS
      CALL PSEUDO
500   CONTINUE
      DO 12 II=1,30
      DO 13 JJ=1,30
      DO 14 KK=1,20
      ITRAC(II,JJ,KK)=0
14    CONTINUE
13    CONTINUE
12    CONTINUE
      MAXH=1
      DO 8 II=1,30
      DO 9 JJ=1,30
      H(II,JJ)=0
      EPS(II,JJ)=0.
      LAYER(II,JJ)=0
9     CONTINUE
8     CONTINUE
      READ(5,PARAM)
      IF(EOF(5)) 600,601
```

```
600      WRITE(6,603)
603      FORMAT(1X,28HEND OF FILE ENCOUNTERED-HELP    )
         CALL CALPLT(0.0,0.0,999)
         STOP   6666
601      CONTINUE
         LL1=
         M2=M*M
         LL2=2+M
         CALL SETUP(MOS,NOS,PHS1,UOS,UMS,TREF,PHSO ,J,ALPHA2,ALPHA3)
         PHS2=ALPHA2*PHS1
         PHS3=ALPHA3*PHS1
         CALL SETUP(MO,NO,PHI1,UO ,UM,TREF,PHIO,J,ALPHA2,ALPHA3)
         PHI2=ALPHA2*PHI1
         PHI3=ALPHA3*PHI1
C        M=SIDE OF SQUARE ARRAY M MAX=60
         TMIG=0
         XLAM=RD*DELT
         IEVAP=0
         ICREAT=0
C        INITIALIZE SUBSTRATE GEOMETRY AND POTENTIALS
         DO 11 JJ=1,30
         DO 10 II=1,30
10       LAYER(II,JJ)=0
11       CONTINUE
         CALL INITIAL
         EMEAN=T*(8.62E-5)
         QD=UM-UO-PHIO
         WRITE(6,399)
         WRITE(6,400)  J,DELT,RD,T,M
         WRITE(6,401)  M2 ,XLAM     ,EMEAN,TSNAP,TSTOP
         WRITE(6,402)  PHI1,PHI2,PHI3,PHIO,ALPHA2
         WRITE(6,403)  PHS1,PHS2,PHS3,PHSO,ALPHA3
         WRITE(6,404)  UO,UM,UE,A,U1
         WRITE(6,405)  UOS,UMS,UES,AS,QD
         WRITE(6,407)MO,NO,MOS,NOS
         WRITE(6,406)  FBB,FAA,D,DS
407      FORMAT(T5,3HMO=,I3,T15,3HNO=,I3,T25,4HMOS=,I3,T35,4HNOS=,I3)
399      FORMAT(1X,15HPARAMETERS ARE: )
400      FORMAT(T10,2HJ=,I3,T34,5HDELT=,1PE14.7,T63,3HRD=,0PF7.1,T91,2HT=,
        1F8.1,T118,2HM=,I5)
401      FORMAT(T6,6H M2   =,I6   ,T33,6HXLAM =,E14.6,T60,6HEMEAN=,F8.4,T90,
        16HTSNAP=,F5.3,T114,6HTSTOP=,F7.1 )
402      FORMAT(T7,5HPHI1=,F10.4,T34,5HPHI2=,F10.4,T61,5HPHI3=,F10.4,T88,
        15HPHIO=,F10.4,T113,7HALPHA2=,F10.4)
403      FORMAT(T7,5HPHS1=,F10.4,T34,5HPHS2=,F10.4,T61,5HPHS3=,F10.4,T88,
        15HPHSO=,F10.4,T112,7HALPHA3=,F10.4  )
404      FORMAT(T9,3HUO=,F10.4,T36,3HUM=,F10.4,T63,3HUE=,F10.4,T91,2HA=,
        1F10.4 ,T115,5HHADS=,F7.3 )
405      FORMAT(T8,4HUOS=,F10.4,T35,4HUMS=,F10.4,T62,4HUES=,F10.4,T90,
```

```
        13HAS=,F10.4 ,T117,3HQD=,F7.3)
406     FORMAT(T10,4HFBB=,9(2X,F8.4),/,T9,4HFAA=,9(2X,F8.4),/,T10,2HD=,
        19(2X,F8.4),/,T9,3HDS=,9(2X,F8.4),/// )
        WRITE(6,408)FAB,FBA
408     FORMAT(T10,4HFAB=,9(2X,F8.4),/,T10,4HFBA=,9(2X,F8.4))
        WRITE(6,308)
308     FORMAT(1H1)
        CALL STOFIN(0,TSTOP)
        GO TO 500
        END
        SUBROUTINE GROW(ITHREE)
        COMMON/BLK5/LAYER(30,30)
        DIMENSION X1(4),X2(4),Y1(4),Y2(4)
        SF=20./3.
        X1(3)=0.
        Y1(3)=0.
        X1(4)=SF
        Y1(4)=SF
        X2(3)=0.
        Y2(3)=0.
        X2(4)=SF
        Y2(4)=SF
        IF(ITHREE.EQ.1) CALL  CALPLT(0.0,12.0,-3)
        FS=3./20.
        IF(ITHREE.EQ.1)GO TO 1
        CALL CALPLT(0.0,-4.0,-3)
        GO TO 4
1       CALL CALPLT(0.0,-3.0,-3)
4       CONTINUE
        CALL GRID(0.0,0.0,FS,FS,20,20)
C       GRID COMPLETE SHADE IN LEVELS
        DO 10 II=3,22
        DO 15 JJ=3,22
        IH=MOD(LAYER(II,JJ),4)
        IF(IH.EQ.3)GO TO 15
        X1(1)=II-3
        Y1(1)=JJ-2
        X1(2)=II-2
        Y1(2)=JJ-2
        X2(1)=II-3
        Y2(1)=JJ-3
        X2(2)=II-2
        Y2(2)=JJ-3
C       SHADE AREA BTWN POINTS
        INT=1+IH+2*(IH-1)*IH
        CALL HAFTONE(X1,Y1,2,X2,Y2,2,INT)
15      CONTINUE
10      CONTINUE
        IF(ITHREE.LT.3)RETURN
```

```
        CALL NFRAME
        ITHREE=0
        RETURN
        END
        SUBROUTINE SETUP(MO,NO,APHI,AUO,AUM,AT,APH ,JA,ALPHA2,ALPHA3)
        PHIO=APH
        J=JA
        UO=AUO
        UM=AUM
        T=AT
        R1=1./SQRT(2.)
        R2=1./SQRT(3.)
        R3=FLOAT(NO)/FLOAT(MO)
        A21=(R1**NO)-R3*(R1**MO)
        A31=(R2**NO)-R3*(R2**MO)
        D1=1.-R3
        A2=A21/D1
        A3=A31/D1
        IF(J.EQ.2)GO TO 111
        IF(J.EQ.3)GO TO 110
C       100 FACE
        ALPHA2=A2
        ALPHA3=0.
        PHI1=PHIO/(1.+ALPHA2)
        PHI1=PHI1/4.
        GO TO 12
111     ALPHA2=A3
        ALPHA3=0.
        PHI1=PHIO/(6.+2.*ALPHA2)
        GO TO 12
110     ALPHA2=A2
        ALPHA3=A3
        PHI1=PHIO/(2.*(1.+ALPHA2)+4.*ALPHA3)
12      CONTINUE
        PHI1=-PHI1
        APHI=PHI1
        RETURN
        END
        SUBROUTINE FACE(F,D,A,J,PHI1,PHI2,PHI3,PHIO,EVIB,T)
        DIMENSION F(9),D(9)
        A2=A/SQRT(2.)
        A3=A/SQRT(2./3.)
C       PHI1,PHI2,PHI3 SHOULD BE NEGATIVE
C       J=1,2 OR 3
        IF(J.EQ.3) GO TO 110
        IF(J.EQ.2) GO TO 111
100     DO 16 IJ=1,4
        IK=2*IJ-1
        IL=2*IJ
```

```
         D(IK)=A
         D(IL)=A2
         F(IK)=PHI2
16       F(IL)=PHI1
         F(9)=PHIO
         GO TO 10
111      DO 17 IJ=2,4
         D(IJ)=A2
         D(IJ+4)=A2
         F(IJ)=PHI1
17       F(IJ+4)=PHI1
         D(1)=A3
         D(5)=A3
         F(1)=PHI2
         F(5)=PHI2
         F(9)=PHIO
         GO TO 10
110      DO 18 IJ=1,4
         IK=2*IJ-1
         D(IK)=A3
18       F(IK)=PHI3
         D(2)=A2
         D(6)=A2
         D(4)=A
         D(8)=A
         F(2)=PHI1
         F(6)=PHI1
         F(4)=PHI2
         F(8)=PHI2
         F(9)=PHIO
10       CONTINUE
         EVIB=T*(8.62E-5)
         D(9)=0.
         RETURN
         END
         SUBROUTINE INITIAL
         COMMON/BLK1/H,EPS(30,30),ITRAC(30,30,20)
         COMMON/BLK2/UO,UM,UE,UOS,UMS,UES,DELT
         COMMON/BLK3/XLAM,TSNAP,M,T,TMIG,IEVAP,ICREAT
         COMMON/BLK4/FAA(9),D(9),FAB(9),FBA(9),DS(9),FBB(9)
         COMMON/BLK5/LAYER(30,30)
         COMMON/BLK6/N1,N2,LETA,M2,LAST
         COMMON/BLK7/PHI1,PHI2,PHI3,PHIO,J,PHS1,PHS2,PHS3,PHSO
         COMMON/BLK8/ISWTCH
         COMMON/BLK9/A,AS,EVIB,EVIBS,RD
         COMMON/BLK10/LL1,LL2,U1,MAXH,TA,TB
C        M=ARRAY SIZE
C        INITIALIZE SUBSTRATE GEOMETRY AND HEIGHTS H
         INTEGER H(30,30)
```

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```
      DO 312 IK=1,30
      DO 311 IJ=1,30
      ITRAC(IK,IJ,1)=0
311   H(IJ,IK)=1
312   CONTINUE
      CALL FACE(FAA,DS,AS,J,PHS1,PHS2,PHS3,PHSO,EVIBS,T)
      CALL FACE(FBB,D,A,J,PHI1,PHI2,PHI3,PHIO,EVIB,T)
C     CHECK SIGNS ON POTENTIALS
      DO 20 II=1,9
      FBA(II)=FAA(II)
      FAB(II)=FBB(II)
20    CONTINUE
      FBA(9)=FAA(9)+UO-UOS
      FAB(9)=FBB(9)+UOS-UO
      DO 41 IK=1,30
      DO 40 IJ=1,30
40    EPS(IJ,IK)=UOS
41    CONTINUE
      ITYPE=0
C      ITYPE=0   SUBSTRATE MATERIAL A-TYPE
C      ITYPE=1   GROWING MATERIAL B-TYPE
C     FLAT SURFACE FOR NOW
C     THIS IS THE PLACE TO PUT IN GEOMETRY CHANGES INITIALIZING SUBSTRATE
C     RADIUS OF CURVATURE EXPERIMENT INITIALIZED HERE. EXAMPLE:A LEFT EDGE
C          DO 300 JJ=1,28
C          300   CALL ADATOM(FAA,LL1,JJ)
C     THIS IS THE PLACE TO PUT IN A TRAP NEAR CENTER  EPS(10,10)=UOS-TRAP
C     FAA CORRECTED FOR FIRST LAYER ADDITION ONLY AFTER FIRST LAYER BUILD UP
      WRITE(6,100)
100   FORMAT(1X,25HINITIAL SUBSTRATE HEIGHTS ,//)
      DO 200 IJ=LL1,LL2
      WRITE(6,101)(H(IJ,I),I=LL1,LL2)
101   FORMAT(10X,20I2)
200   CONTINUE
      DO 201 IJ=LL1,LL2
      WRITE(6,202) (EPS(IJ,I),I=LL1,LL2)
202   FORMAT(10X,20F6.2)
201   CONTINUE
      RETURN
      END
      SUBROUTINE DIFF(II,JJ,DMIG,IN,JN)
      COMMON/BLK1/H,EPS(30,30),ITRAC(30,30,20)
      COMMON/BLK2/UO,UM,UE,UOS,UMS,UES,DELT
      COMMON/BLK3/XLAM,TSNAP,M,T,TMIG,IEVAP,ICREAT
      COMMON/BLK4/FAA(9),D(9),FAB(9),FBA(9),DS(9),FBB(9)
      COMMON/BLK5/LAYER(30,30)
      COMMON/BLK7/PHI1,PHI2,PHI3,PHIO,J,PHS1,PHS2,PHS3,PHSO
      COMMON/BLK8/ISWTCH
      COMMON/BLK10/LL1,LL2,U1,MAXH,TA,TB
```

40

```
      DIMENSION IV(8,2),IS(8,2),WW(8),Q(8)
          INTEGER W(8)
      INTEGER H(30,30)
      IC=0
C     F.NDOM WALK FROM SITE I TO NI
          DMIG=0.
C     FIND AVAILABLE SITES (IF ANY)
C     IS(8) IS LIST OF SAVED AVAILABLE SITES, IC IS NUMBER OF SITES
      DO 10 YJK=1,8
      W(IJK)=0.
10    CONTINUE
C     REMOVE ADATOM
      IJK=H(II,JJ)
      IF(IJK.LE.0)ITYPER=0
      IF(IJK.LE.0)GO TO 20
      ITYPER=ITRAC(II,JJ,IJK)
20    CONTINUE
      CALL SUBATOM(II,JJ,ITYPER)
      CALL XYX
      JJ1=JJ+1
      JJO=JJ-1
      III=II+1
      IIO=II-1
      IF(JJ1.GT.22)JJ1=3
      IF(JJO.LT.3)JJO=22
      IF(II1.GT.22)II1=3
      IF(IIO.LT.3)IIO=22
C     FIND AVAILABLE MIGRATION SITES
      IQ=H(II,JJ)+1
      Q(1)=IQ-H(II,JJ1)
      IF(Q(1).LE.0)GO TO 400
      IC=IC+1
      IS(IC,1)=II
      IS(IC,2)=JJ1
      CALL PBOND(II,JJ1,W(IC),J)
400   Q(2)=IQ-H(II1,JJ)
      IF(Q(2).LE.0)GO TO 401
      IC=IC+1
      IS(IC,1)=II1
      IS(IC,2)=JJ
      CALL PBOND(II1,JJ,W(IC),J)
401   Q(3)=IQ-H(II,JJO)
      IF(Q(3).LE.0)GO TO 402
      IC=IC+1
      IS(IC,1)=II
      IS(IC,2)=JJO
      CALL PBOND(II,JJO,W(IC),J)
402   Q(4)=IQ-H(IIO,JJ)
      IF(Q(4).LE.0)GO TO 40?
```

```
        IC=IC+1
        CALL PBOND(IIO,JJ,W(IC),J)
        IS(IC,1)=IIO
        IS(IC,2)=JJ
403     Q(5)=IQ-H(IIO,JJ1)
        IF(Q(5).LE.0)GO TO 404
        IC=IC+1
        IS(IC,1)=IIO
        IS(IC,2)=JJ1
        CALL PBOND(IIO,JJ1,W(IC),J)
404     Q(6)=IQ-H(II1,JJ1)
        IF(Q(6).LE.0)GO TO 405
        IC=IC+1
        IS(IC,1)=II1
        IS(IC,2)=JJ1
        CALL PBOND(II1,JJ1,W(IC),J)
405     Q(7)=IQ-H(II1,JJO)
        IF(Q(7).LE.0)GO TO 406
        IC=IC+1
        IS(IC,1)=II1
        IS(IC,2)=JJO
        CALL PBOND(II1,JJO,W(IC),J)
406     Q(8)=IQ-H(IIO,JJO)
        IF(Q(8).LE.0)GO TO 407
        IC=IC+1
        IS(IC,1)=IIO
        IS(IC,2)=JJO
        CALL PBOND(IIO,JJO,W(IC),J)
407     CONTINUE
        JL=4+2*(J-1)-3*(J-1)*(J-2)
C       TEST IC
        IF(IC.EQ.0)GO TO 500
C       WEIGHTED RANDOM WALK
        WT=0
         IF(IC.EQ.1)GO TO 100
        DO 408 IM=1,IC
         WT=WT+W(IM)
408     WW(IM)=WT
        DO 409 IM=1,IC
409     WW(IM)=WW(IM)/WT
        R=URAN(0)
        IM=1
411     IF(R.LE.WW(IM))MS=IM
        IF(R.LE.WW(IM))GO TO 412
        IM=IM+1
        IF(IM.EQ.IC)MS=IC
        IF(IM.EQ.IC)GO TO 412
        GO TO 411
412     IN=IS(MS,1)
```

```
          JN=IS(MS,2)
          GO TO 60
100       IN=IS(1,1)
          JN=IS(1,2)
          GO TO 60
500       CONTINUE
C     JUMP TO HIGHER LEVEL ONLY IF RANDOM ENERGY GREATER THAN
C        NEAREST NEIGHBOR BONDS - RANDOM WALK TO NN SITES
          R=URAN(0)
          MSITE=R*JL+2
          IF(MSITE .LE.JL)GO TO 567
C        NO MIGRATION
          IN=II
          JN=JJ
          DMIG=0
570       CALL ADATOM(IN,JN,ITYPER)
          RETURN
567       CONTINUE
          IV(1,1)=II
          IV(1,2)=JJ1
          IV(2,1)=II
          IV(2,2)=JJ0
          IV(3,1)=III1
          IV(3,2)=JJ
          IV(4,1)=II0
          IV(4,2)=JJ
          IV(5,1)=III1
          IV(5,2)=JJ1
          IV(6,1)=II0
          IV(6,2)=JJ0
          IN=IV(MSITE,1)
          JN=IV(MSITE,2)
          DMIG=D(MSITE)
60        CONTINUE
C     TEST FOR MIGRATION OVER BOUNDARIES
          IF(IN.LT.LL1)GO TO 70
          IF(IN.GT.LL2)GO TO 71
          IF(JN.LT.LL1)GO TO 72
          IF(JN.GT.LL2)GO TO 73
          GO TO 80
70        CONTINUE
          IF(JN.EQ.2)GO TO 74
          IF(JN.EQ.23)GO TO 75
          IN=22
          GO TO 80
74        IN=22
          JN=22
          GO TO 80
75        IN=22
```

```
              JN=3
              GO TO 80
71            IF(JN.EQ.2)GO TO 76
              IF(JN.EQ.23)GO TO 77
              IN=3
              GO TO 80
76            IN=3
              JN=22
              GO TO 80
77            IN=3
              JN=3
              GO TO 80
72            IF(IN.EQ.2)GO TO 74
              IF(IN.EQ.23)GO TO 76
              JN=22
              GO TO 80
73            IF(IN.EQ.2)GO TO 75
              IF(IN.EQ.23)GO TO 77
              JN=3
80            CONTINUE
              CALL ADATOM(IN,JN,ITYPER)
                  DMIG=D(2)
              RETURN
              END
              SUBROUTINE PBOND(II,JJ,NNB,JCODE)
              COMMON/BLK1/H,EPS(30,30),ITRAC(30,30,20)
              COMMON/BLK5/LAYER(30,30)
              INTEGER Q(6)
              INTEGER H(30,30)
              NNB=1
                JJ1=JJ+1
                JJ0=JJ-1
                II1=II+1
                II0=II-1
              IQ=H(II,JJ)+1
              IF(JCODE.EQ.3)GO TO 3
              IF(JCODE.EQ.2)GO TO 2
              Q(1)=IQ-H(II,JJ1)
              Q(2)=IQ-H(II1,JJ)
              Q(3)=IQ-H(II,JJ0)
              Q(4)=IQ-H(II0,JJ)
              DO 10 IK=1,4
              IF(Q(IK).LE.0)NNB=NNB+1
10            CONTINUE
              IF(NNB.EQ.5)NNB=1
              RETURN
2             CONTINUE
              Q(1)=IQ-H(II,JJ1)
              Q(2)=IQ-H(II1,JJ1)
```

```
         Q(3)=IQ-H(II1,JJ)
         Q(4)=IQ-H(II,JJO)
         Q(5)=IQ-H(IIO,JJO)
         Q(6)=IQ-H(IIO,JJ)
         DO 20 IK=1,6
         IF(Q(IK).LE.0)NNB=NNB+1
20       CONTINUE
         IF(NNB.EQ.7)NNB=1
         RETURN
3        CONTINUE
         Q(1)=IQ-H(II,JJ1)
         Q(2)=IQ-H(II,JJO)
         DO 30 IK=1,2
         IF(Q(IK).LE.0)NNB=NNB+1
30       CONTINUE
         IF(NNB.EQ.3)NNB=1
         RETURN
         END
         SUBROUTINE ADATOM(I,J,ITYPE)
         COMMON/BLK1/H,EPS(30,30),ITRAC(30,30,20)
         COMMON/BLK4/FAA(9),D(9),FAB(9),FBA(9),DS(9),FBB(9)
         COMMON/BLK5/LAYER(30,30)
         DIMENSION W(9)
         INTEGER H(30,30)
         IF(H(I,J).LE.0)ISPOT=0
         IF(H(I,J).LE.0)GO TO 80
C        GO AHEAD AND ADD NEW ADATOMS THEN CORRECT BOUNDARIES IF NECESSARY
         ISPOT=ITRAC(I,J,H(I,J))
80       CONTINUE
         IF((ISPOT.EQ.0).AND.(ITYPE.EQ.0))GO TO 10
         IF((ISPOT.EQ.0).AND.(ITYPE.EQ.1))GO TO 20
         IF((ISPOT.EQ.1).AND.(ITYPE.EQ.0))GO TO 30
         DO 40 LM=1,9
40       W(LM)=FBB(LM)
         GO TO 100
10       DO 50 LM=1,9
50       W(LM)=FAA(LM)
         GO TO 100
20       DO 60 LM=1,9
60       W(LM)=FBA(LM)
         GO TO 100
30       DO 70 LM=1,9
70       W(LM)=FAB(LM)
100      CONTINUE



         EPS(I,J)=EPS(I,J)+W(9)
```

```
          EPS(I-1,J+1)=EPS(I-1,J+1)+W(1)
          EPS(I,J+1)=EPS(I,J+1)+W(2)
          EPS(I+1,J+1)=EPS(I+1,J+1)+W(3)
          EPS(I+1,J)=EPS(I+1,J)+W(4)
          EPS(I+1,J-1)=EPS(I+1,J-1)+W(5)
          EPS(I,J-1)=EPS(I,J-1)+W(6)
          EPS(I-1,J-1)=EPS(I-1,J-1)+W(7)
          EPS(I-1,J)=EPS(I-1,J)+W(8)
          H(I,J)=H(I,J)+1
          LAYER(I,J)=LAYER(I,J)+1
          ITRAC(I,J,H(I,J))=ITYPE
C         IS ADATOM AT AN EDGE?
          TEST1=(I-4)*(21-I)
          TEST2=(J-4)*(21-J)
          IF((TEST1.LT.0).OR.(TEST2.LT.0))GO TO 2
          IF((TEST1.EQ.0).OR.(TEST2.EQ.0))CALL EDD(I,J)
          RETURN
2         CONTINUE
          CALL EDGE(W,I,J)
          RETURN
          END
          SUBROUTINE SUBATOM(I,J,ITYPE)
          COMMON/BLK1/H,EPS(30,30),ITRAC(30,30,20)
          COMMON/BLK4/FAA(9),D(9),FAB(9),FBA(9),DS(9),FBB(9)
          COMMON/BLK5/LAYER(30,30)
          DIMENSION W(9)
          INTEGER H(30,30)
C         GO AHEAD AND SUBTRACT OLD ADATONS THEN CORRECT BOUNDARIES
          IK=H(I,J)-1
          IF(IK.LE.0)ION=0
          IF(IK.LE.0)GO TO 80
          ION=ITRAC(I,J,IK)
80        CONTINUE
          IF((ION.EQ.0).AND.(ITYPE.EQ.1))GO TO 10
          IF((ION.EQ.0).AND.(ITYPE.EQ.0))GO TO 20
          IF((ION.EQ.1).AND.(ITYPE.EQ.1))GO TO 30
          DO 40 LM=1,9
40        W(LM)=FAA(LM)
          GO TO 100
10        DO 50 LM=1,9
50        W(LM)=FBA(LM)
          GO TO 100
20        DO 60 LM=1,9
60        W(LM)=FAA(LM)
          GO TO 100
30        DO 70 LM=1,9
70        W(LM)=FAB(LM)
100       CONTINUE
```

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```
         EPS(I,J)=EPS(I,J)-W(9)
         EPS(I-1,J+1)=EPS(I-1,J+1)-W(1)
         EPS(I,J+1)=EPS(I,J+1)-W(2)
         EPS(I+1,J+1)=EPS(I+1,J+1)-W(3)
         EPS(I+1,J)=EPS(I+1,J)-W(4)
         EPS(I+1,J-1)=EPS(I+1,J-1)-W(5)
         EPS(I,J-1)=EPS(I,J-1)-W(6)
         EPS(I-1,J-1)=EPS(I-1,J-1)-W(7)
         EPS(I-1,J)=EPS(I-1,J)-W(8)
         ITRAC(I,J,H(I,J))=-1
         H(I,J)=H(I,J)-1
         LAYER(I,J)=LAYER(I,J)-1
C        IS ADATOM AT AN EDGE?
         TEST1=(I-4)*(21-I)
         TEST2=(J-4)*(21-J)
         IF((TEST1.LT.0).OR.(TEST2.LT.0))GO TO 2
         IF((TEST1.EQ.0).OR.(TEST2.EQ.0))CALL EDD(I,J)
         RETURN
2        CONTINUE
         CALL EDGE(W,I,J)
         RETURN
         END
         SUBROUTINE RANDOM(XO,X1,RN)
C        XO IS SEED SUPPLIED BY USER
         INTEGER XO,AA,MP,X1
         AA=3125
         MP=34359738337
         X1=MOD(XO*AA,MP)
         RN=FLOAT(X1)/FLOAT(MP)
         XO=X1
         RETURN
         END
         SUBROUTINE EDGE(W,I,J)
         COMMON/BLK1/H,EPS(30,30),ITRAC(30,30,20)
         DIMENSION W(9)
         INTEGER H(30,30)
C        ADJUST FOR EDGE EFFECTS CASES WHERE I=3,22,J=3,22
         IF(I.EQ.3)GO TO 20
         IF(I.EQ.22)GO TO 25
         IF(J.EQ.3)GO TO 30
         IF(J.EQ.22)GO TO 35
         RETURN
20       CONTINUE
C        TOP EDGE I=3
         IF(J.EQ.3)GO TO 21
         IF(J.EQ.22)GO TO 22
```

```
      EPS(22,J-1)=EPS(2,J-1)
      EPS(22,J)=EPS(2,J)
      EPS(22,J+1)=EPS(2,J+1)
      EPS(23,J-1)=EPS(3,J-1)
      EPS(23,J)=EPS(3,J)
      EPS(23,J+1)=EPS(3,J+1)
      H(23,J)=H(3,J)
      RETURN
21    EPS(22,22)=EPS(2,2)
      EPS(2,22)=EPS(2,2)
      EPS(22,2)=EPS(2,2)
      EPS(2,23)=EPS(2,3)
      EPS(22,23)=EPS(2,3)
      EPS(22,3)=EPS(2,3)
      EPS(22,4)=EPS(2,4)
      EPS(23,4)=EPS(3,4)
      EPS(3,23)=EPS(3,3)
      EPS(23,23)=EPS(3,3)
      EPS(23,3)=EPS(3,3)
      EPS(4,23)=EPS(4,3)
      EPS(4,22)=EPS(4,2)
      EPS(3,22)=EPS(3,2)
      EPS(23,2)=EPS(3,2)
      EPS(23,22)=EPS(3,2)
      H(3,23)=H(3,3)
      H(23,23)=H(3,3)
      H(23,3)=H(3,3)
      RETURN
22    CONTINUE
      H(23,22)=H(3,22)
      H(23,2)=H(3,22)
      H(3,2)=H(3,22)
      EPS(22,21)=EPS(2,21)
      EPS(23,21)=EPS(3,21)
      EPS(2,2)=EPS(2,22)
      EPS(22,2)=EPS(2,22)
      EPS(22,22)=EPS(2,22)
      EPS(22,23)=EPS(2,23)
      EPS(22,3)=EPS(2,23)
      EPS(2,3)=EPS(2,23)
      EPS(23,23)=EPS(3,23)
      EPS(23,3)=EPS(3,23)
      EPS(3,3)=EPS(3,23)
      EPS(23,22)=EPS(3,22)
      EPS(23,2)=EPS(3,22)
      EPS(3,2)=EPS(3,22)
      EPS(4,3)=EPS(4,23)
      EPS(4,2)=EPS(4,22)
      RETURN
```

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```
 25     CONTINUE
 C      BOTTOM EDGE I=22
        IF(J.EQ.3)GO TO 26
        IF(J.EQ.22)GO TO 27
        EPS(2,J-1)=EPS(22,J-1)
        EPS(3,J-1)=EPS(23,'-1)
        EPS(3,J)=EPS(23,J)
        EPS(2,J)=EPS(22,J)
        EPS(3,J+1)=EPS(23,J+1)
        EPS(2,J+1)=EPS(22,J+1)
        H(2,J)=H(22,J)
        RETURN
 26     CONTINUE
        H(22,23)=H(22,3)
        H(2,3)=H(22,3)
        H(2,23)=H(22,3)
        EPS(21,22)=EPS(21,2)
        EPS(21,23)=EPS(21,3)
        EPS(2,4)=EPS(22,4)
        EPS(3,4)=EPS(23,4)
        EPS(3,3)=EPS(23,3)
        EPS(3,23)=EPS(23,3)
        EPS(23,23)=EPS(23,3)
        EPS(3,2)=EPS(23,2)
        EPS(3,22)=EPS(23,2)
        EPS(23,22)=EPS(23,2)
        EPS(2,2)=EPS(22,2)
        EPS(2,22)=EPS(22,2)
        EPS(22,22)=EPS(22,2)
        EPS(2,3)=EPS(22,3)
        EPS(2,23)=EPS(22,3)
        EPS(22,23)=EPS(22,3)
        H(2,22)=H(22,22)
        H(2,2)=H(22,22)
        H(22,2)=H(22,22)
        RETURN
 27     CONTINUE
        EPS(21,2)=EPS(21,22)
        EPS(21,3)=EPS(21,23)
        EPS(22,3)=EPS(22,23)
        EPS(2,3)=EPS(22,23)
        EPS(2,23)=EPS(22,23)
        EPS(23,3)=EPS(23,23)
        EPS(3,3)=EPS(23,23)
        EPS(3,23)=EPS(23,23)
        EPS(23,2)=EPS(23,22)
        EPS(3,2)=EPS(23,22)
        EPS(3,22)=EPS(23,22)
        EPS(3,21)=EPS(23,21)
```

```
          EPS(2,21)=EPS(22,21)
          EPS(22,2)=EPS(22,22)
          EPS(2,2)=EPS(22,22)
          EPS(2,22)=EPS(22,22)
          RETURN
30        CONTINUE
          IF(I.EQ.3)GO TO 21
          IF(I.EQ.22)GO TO 26
          H(I,23)=H(I,3)
          EPS(I-1,23)=EPS(I-1,3)
          EPS(I,23)=EPS(I,3)
          EPS(I+1,23)=EPS(I+1,3)
          EPS(I-1,22)=EPS(I-1,2)
          EPS(I,22)=EPS(I,2)
          EPS(I+1,22)=EPS(I+1,2)
          RETURN
35        CONTINUE
          IF(I.EQ.3)GO TO 22
          IF(I.EQ.22)GO TO 27
          H(I,2)=H(I,22)
          EPS(I-1,3)=EPS(I-1,23)
          EPS(I,3)=EPS(I,23)
          EPS(I+1,3)=EPS(I+1,23)
          EPS(I-1,2)=EPS(I-1,22)
          EPS(I,2)=EPS(I,22)
          EPS(I+1,2)=EPS(I+1,22)
          RETURN
          END
          SUBROUTINE EDD(I,J)
          COMMON/BLK1/H,EPS(30,30),ITRAC(30,30,20)
          INTEGER H(30,30)
          IF(I.EQ.4)GO TO 20
          IF(I.EQ.21)GO TO 25
          IF(J.EQ.4)GO TO 30
          IF(J.EQ.21)GO TO 35
20        CONTINUE
          IF(J.EQ.4) GO TO   21
          IF(J.EQ.21)GO TO 22
          EPS(23,J+1)=EPS(3,J+1)
          EPS(23,J)=EPS(3,J)
          EPS(23,J-1)=EPS(3,J-1)
          RETURN
21        EPS(3,23)=EPS(3,3)
          EPS(4,23)=EPS(4,3)
          EPS(5,23)=EPS(5,3)
          EPS(23,23)=EPS(3,3)
          EPS(23,3)=EPS(3,3)
          EPS(23,4)=EPS(3,4)
          EPS(23,5)=EPS(3,5)
```

```
         RETURN
22       EPS(3,2)=EPS(3,22)
         EPS(4,2)=EPS(4,22)
         EPS(5,2)=EPS(5,22)
         EPS(23,2)=EPS(3,22)
         EPS(23,20)=EPS(3,20)
         EPS(23,21)=EPS(3,21)
         EPS(23,22)=EPS(3,22)
         RETURN
25       CONTINUE
         IF(J.EQ.4)GO TO 26
         IF(J.EQ.21)GO TO 27
         EPS(2,J-1)=EPS(22,J-1)
         EPS(2,J)=EPS(22,J)
         EPS(2,J+1)=EPS(22,J+1)
         RETURN
26       EPS(2,3)=EPS(22,3)
         EPS(2,4)=EPS(22,4)
         EPS(2,5)=EPS(22,5)
         EPS(2,23)=EPS(22,3)
         EPS(20,23)=EPS(20,3)
         EPS(21,23)=EPS(21,3)
         EPS(22,23)=EPS(22,3)
         RETURN
27       EPS(22,2)=EPS(22,22)
         EPS(21,2)=EPS(21,22)
         EPS(20,2)=EPS(20,22)
         EPS(2,2)=EPS(22,22)
         EPS(2,20)=EPS(22,20)
         EPS(2,21)=EPS(22,21)
         EPS(2,22)=EPS(22,22)
         RETURN
30       IF(I.EQ.4)GO TO 21
         IF(I.EQ.21)GO TO 26
         EPS(I-1,23)=EPS(I-1,3)
         EPS(I,23)=EPS(I,3)
         EPS(I+1,23)=EPS(I+1,3)
         RETURN
35       IF(I.EQ.4)GO TO 22
         IF(I.EQ.21)GO TO 27
         EPS(I-1,2)=EPS(I-1,22)
         EPS(I,2)=EPS(I,22)
         EPS(I+1,2)=EPS(I+1,22)
         RETURN
         END
         SUBROUTINE STOFIN(TSTART,TSTOP)
         COMMON/BLK1/H,EPS(30,30),ITRAC(30,30,20)
         COMMON/BLK2/UO,UM,UE,UOS,UMS,UES,DELT
         COMMON/BLK3/XLAM,TSNAP,N,T,TMIG,IEVAP,ICREAT
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      COMMON/BLK4/FAA(9),D(9),FAB(9),FBA(9),DS(9),FBB(9)
      COMMON/BLK5/LAYER(30,30)
      COMMON/BLK6/N1,N2,LETA,M2,LAST
      COMMON/BLK7/PHI1,PHI2,PHI3,PHIO,J,PHS1,PHS2,PHS3,PHSO
      COMMON/BLK8/ISWTCH
      COMMON/BLK9/A,AS,EVIB,EVIBS,RD
      COMMON/BLK10/LL1,LL2,U1,MAXH,TA,TB
C     VALUES OF PARAMETERS COME VIA COMMON STATEMENTS
      INTEGER H(30,30)
      DIMENSION  IYMIG(400,3)
      DIMENSION IRSIT(300,3)
      DIMENSION IKC(20,2),  IV(401)
      DIMENSION DC(400),HTS(10)
      ITIME=1.0
      ITHREE=1
      IF(ISWTCH.EQ.0)GO TO 6
      CALL GROW(ITHREE)
6     CONTINUE
      ITHREE=ITHREE+1
      IRPLUS=0
      IMIGR=0
      DO 504 JJ=1,3
      DO 503 II=1,400
      IYMIG(II,JJ)=0
503   CONTINUE
504   CONTINUE
      TTIME=TSTART
      UEVAP=UE
      UMIGR=UM
      ICOUNT=0
      IOUT=0
      PROBC=0.
      PROBE=0.
      PROBM=0.
C     IBULK IS BULK DIFFUSION COUNTER-REMOVE ADATOMS FROM SURFACE
      IBULK=0
      WT1=2.
C     WT1 IS WEIGHT FOR BULK DIFFUSION
C     QB IS BULK DIFFUSION ENERGY BARRIER
      XKT=T*(8.62E-5)
      TOUT=TSNAP
      QD=UM-UO-PHIO
      TAUD=(1.0E-12)*EXP(QD/XKT)
C     TAUD IS THE MEAN TIME BETWEEN HOPS
C     NHOP IS THE NO. OF HOPS IN DELT SECONFAA
2     XNHOP=DELT/TAUD
      XNSAMP=(1.0E12)*TAUD
      XNOFP=(1.0E12)*DELT
      XNSCAN=TOUT/DELT
```

```
          QB=WT1*QD
          UBULK=UO+PHIO+QB
          IF(UBULK.GE.UE)UBULK=UE-.001
          TT1=1./(1.+WT1)
          XNTOUT=TOUT-DELT/2.
C         INITIALIZE TIME COUNTER FOR CASE WHERE IJK=0
          TINIT=DELT/2.
          XXLAM=XLAM/DELT
C         XXLAM IS REALLY RD=DEPOSITION RATE
1         XIJK=XLAM
          IJK=XIJK
C         IJK IS NUMBER OF RANDOM DEPOSITIONS DURING DELT
C         IF DELT IS VERY SMALL XIJK IS ALWAYS LESS THAN ONE AND HENCE IJK=0
C         IN CASE IJK=0 GO TO 700 SCAN SURFACE AND PERFORM MIGRATIONS/EVAPORATIONS
C         DURING THE DELT INTERVAL AND THEN RETURN TO 1
C         UPDATE TINIT IF IJK =0
          IF(IJK .EQ. 0) TINIT=TINIT+DELT
C         HAS ENOUGH TIME ELAPSED FOR THE ADDITION OF ONE ADATOM?
          XXIJK=XXLAM*TINIT
          IXIJK=XXIJK
          IF(IXIJK .GT.0)IJK=IXIJK
          IF(IJK.GT.0)TINIT=DELT/2.
C         IF  DEPOSITION RATE IS ZERO GO TO 700 SCAN SURFACE
          IF(XLAM .LE. 0.)GO TO 700
          IF(IJK .EQ. 0) GO TO 700
          IRPLUS=IRPLUS+IJK
          CALL URNS(IJK,IRSIT,M)
          DO 500 IL=1,IJK
C         ADD THERMALLY ACCOMODATED ADATOMS
          IRS=IRSIT(IL,1)
          JCS=IRSIT(IL,2)
          ITYPE=IRSIT(IL,3)
          CALL ADATOM(IRS,JCS,ITYPE)
500       CONTINUE
700       CONTINUE
          IX=0
          IY=0
          IZ=0
          IB=0
C         IF LAYER IS 1 THEN UOS,UMS,UES DOMINATES
C         CREATION, MIGRATION, EVAPORATION
C         NOW DO ALL MIGRATIONS FOR SITES WITH FLAGS
          NSCAN=0
          DO 502 JJ1=LL1,LL2
          DO 501 II1=LL1,LL2
          IF(EPS(II1,JJ1).GT.UMIGR)GO TO 25
          IF(LAYER(II1,JJ1).LE.0)GO TO 501
          RAN=URAN(0)
          ABC=-ALOG(RAN)/XNOFP
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          ENGY=-XKT*ALOG(ABC)
          U=EPS(II1,JJ1)+ENGY
          IF(U.LT.UMIGR)GO TO 30
          IF(U.LT.UBULK)GO TO 25
          IF(U.LT.UE)GO TO 16
          GO TO 20
   16     IF(RAN.GT.TT1)GO TO 25
          IB=IB+1
          GO TO 20
   C      MIGRATION OCCURS
   25     IY=IY+1
          NSCAN=NSCAN+1
          IYMIG(NSCAN,1)=II1
          IYMIG(NSCAN,2)=JJ1
          IYMIG(NSCAN,3)=1
          GO TO 501
   C      EVAPORATION
   20     IZ=IZ+1
          NSCAN=NSCAN+1
          IYMIG(NSCAN,1)=II1
          IYMIG(NSCAN,2)=JJ1
          IYMIG(NSCAN,3)=0
          GO TO 501
   30     IX=IX+1
   501        CONTINUE
   502     CONTINUE
          ICOUNT=ICOUNT+1
          TOTAL=IX+IY+IZ
          ICREAT=ICREAT+IX
          IEVAP=IEVAP+IZ-IB
          IMIGR=IMIGR+IY
          IBULK=IBULK+IB
          IF(NSCAN.EQ.0)GO TO 506
          CALL MIXUP(IV,NSCAN)
          DO 505 IK=1,NSCAN
          IJ=IV(IK)
          II1=IYMIG(IJ,1)
          JJ1=IYMIG(IJ,2)
          ITYPE=IYMIG(IJ,3)
          IF(ITYPE.EQ. 0)GO TO 508
          CALL DIFF(II1,JJ1,DMIG,NI1,NJ1)
          TMIG=TMIG+DMIG
          GO TO 505
   508    CONTINUE
          ITYR=0
          IF(H(II1,JJ1).LE.0)GO TO 70
          ITYR=ITRAC(II1,JJ1,H(II1,JJ1))
   70     CONTINUE
          CALL SUBATOM(II1,JJ1,ITYR)
```

54

```
505     CONTINUE
506     CONTINUE
        TTIME=TTIME+DELT
C       OUTPUT EVERY TOUT SECONDS
        IF(TTIME .GE. XNTOUT) GO TO 652
        GO TO 1
652     CONTINUE
        XNTOUT=TTIME+TOUT-DELT/2.
C       BEFORE STOPPING DO AVERAGES FOR THIS DELT RUN
C       RE IN UNITS OF ADATOMS/SEC  TO CONVERT TO NM/SEC MULTIPLY BY(.1*A)/400
C       RE=EVAPORATION RATE
        RE=FLOAT(IEVAP)/TTIME
C       RG=AVG GROWTH RATE IN NM/SEC
        RG=A*(FLOAT(IRPLUS-IEVAP-IBULK))/FLOAT(M2)
        RG=.1*RG/TTIME
C       RG IN UNITS OF NM/SEC
C       RF=ROUGHNESS FACTOR ;   EBAR=AVG POTENTIAL WELL
        EBAR=0
        DO 100 II=LL1,LL2
        DO 101 JJ=LL1,LL2
        EBAR=EBAR+EPS(II,JJ)
101     CONTINUE
100     CONTINUE
        EBAR=EBAR/FLOAT(M2)
        PF=ABS((UO-EBAR)/UO)*100
C       PF IS ROUGHNESS FACTOR BY WAY OF POTENTIAL DEVIATION FROM NORM
        XN=ICOUNT
        CALL UPDATE(RF,THETA,TH2,DC,HTS,J)
        IF(ISWTCH.EQ.0)GO TO 5
        CALL GROW(ITHREE)
5       CONTINUE
        ITHREE=ITHREE+1
        N=XN
        ICC=0
        DO 50 II=1,400
        IF(DC(II).EQ.0)GO TO 50
        IF(ICC.GT.20)GO TO 50
        ICC=ICC+1
        IKC(ICC,1)=II
        IKC(ICC,2)=DC(II)
50      CONTINUE
        WRITE(6,298)TTIME,((IKC(II,JJ),JJ=1,2),II=1,ICC)
298     FORMAT(1X,6HTTIME=,F8.3,5X,37HDENSITY OF CLUSTERS (SIZE,FREQUENCY)
     1   ,/,T20,(10(1H(,I3,1H,,I3,1H),2X)),/,T20,(10(1H(,I3,1H,,I3,1H),2X
     2)))
        WRITE(6,299) (LAYER(3,JJ),JJ=3,22),(LAYER(3,JJ),JJ=3,22),N,J,XNHOP
299     FORMAT(10X,40I1,T60,6H    N= ,I9 ,T80,5H   J= ,I2,T100,5HNHOP=,
     1E14.7)
        WRITE(6,300)(LAYER(4,JJ),JJ=3,22),(LAYER(4,JJ),JJ=3,2?):,IMIGR,
```

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```
      1ICREAT,IEVAP,IBULK
300   FORMAT(10X,40I1,T60,6HIMIGR=,I9,T80,7HICREAT=,I9,T100,6HIEVAP=,I9,
      1T120,6HIBULK=,I6)
      WRITE(6,301)(LAYER(5,JJ),JJ=3,22),(LAYER(5,JJ),JJ=3,22),THETA,TH2,
      1TAUD,TA
301   FORMAT(10X,40I1,T60,9HTHETA(1)=,F8.4,T80,9HTHE.A(2)=,F8.3,T100,
      15HTAUD=,E14.5,T122,3HTA=,F5.0)
      WRITE(6,302)(LAYER(6,JJ),JJ=3,22),(LAYER(6,JJ),JJ=3,22),IRPLUS,
      1XNHOP,TMIG,TB
302   FORMAT(10X,40I1,T60,7HIRPLUS=,I9,T80,5HNHOP=,E14.7,T100,5HTMIG=,
      1E14.7,T122,3HTB=,F5.0)
      WRITE(6,303)(LAYER(7,JJ),JJ=3,22),(LAYER(7,JJ),JJ=3,22),RE,RG,RF
303   FORMAT(10X,40I1,T60,3HRE=,F9.4,T80,3HRG=,F9.4,T100,3HRF=,F9.4)
      WRITE(6,304)(LAYER(8,JJ),JJ=3,22),(LAYER(8,JJ),JJ=3,22),XNOFP,
      1EBAR,XNSAMP
304   FORMAT(10X,40I1,T60,5HNOFP=,E14.7,T80,5HEBAR=,F8.3,2X,
      110HNSAMPPHOP=,E14.7)
      WRITE(6,310)(LAYER(9,JJ),JJ=3,22),(LAYER(9,JJ),JJ=3,22),HTS
310   FORMAT(10X,40I1,T60,4HHTS=,10F4.0 )
      DO 201 II=10,22
      WRITE(6,305)(LAYER(II,JJ),JJ=3,22),(LAYER(II,JJ),JJ=3,22)
305   FORMAT(10X,40I1)
201   CONTINUE
      IOUT=IOUT+1
      ITEST1=MOD(IOUT,2)
      IF(ITEST1.EQ.0)GO TO 60
      WRITE(6,306)
306   FORMAT( /)
      GO TO 61
60    CONTINUE
      WRITE(6,311)
311   FORMAT(1H1)
61    CONTINUE
      IF(TTIME.GE.TSTOP)GO TO 876
      IF((TTIME+DELT/2.).LT. TSTOP) GO TO 1
876   CONTINUE
      IF(ISWTCH.EQ.1) CALL NFRAME
      RETURN
      END
      SUBROUTINE XYX
      COMMON/BLK1/H,EPS(30,30),ITRAC(30,30,20)
      COMMON/BLK5/LAYER(30,30)
C     UPDATE FRINGES OF PERIODIC PATTERN
      INTEGER H(30,30)
      DO 6 I=3,22
      LAYER( 1, I)=LAYER(21, I)
      H(1,I)=H(21,I)
      LAYER( 2, I)=LAYER(22, I)
      H(2,I)=H(22,I)
```

```
      LAYER(23,I )=LAYER( 3, I)
      H(23,I)=H(3,I)
      LAYER(24, I)=LAYER( 4, I)
      H(24,I)=H(4,I)
      LAYER( I, 1)=LAYER( I,21)
      H(I,1)=H(I,21)
      LAYER( I, 2)=LAYER( I,22)
      H(I,2)=H(I,22)
      LAYER( I,23)=LAYER( I,3 )
      H(I,23)=H(I,3)
      LAYER( I,24)=LAYER( I, 4)
      H(I,24)=H(I,4)
6     CONTINUE
C     CORNERS UPDATED
      LAYER( 1, 1)=LAYER(21,21)
      H(1,1)=H(21,21)
      LAYER( 1, 2)=LAYER(21,22)
      H(1,2)=H(21,22)
      LAYER( 2, 1)=LAYER(22,21)
      H(2,1)=H(22,21)
      LAYER( 2, 2)=LAYER(22,22)
      H(2,2)=H(22,22)
      LAYER(23, 1)=LAYER( 3,21)
      H(23,1)=H(3,21)
      LAYER(23, 2)=LAYER( 3,22)
      H(23,2)=H(3,22)
      LAYER(24, 1)=LAYER( 4,21)
      H(24,1)=H(4,21)
      LAYER(24, 2)=LAYER( 4,22)
      H(24,2)=H(4,22)
      LAYER( 1,23)=LAYER(21, 3)
      H(1,23)=H(21,3)
      LAYER( 1,24)=LAYER(21,4 )
      H(1,24)=H(21,4)
      LAYER( 2,23)=LAYER(22, 3)
      H(2,23)=H(22,3)
      LAYER( 2,24)=LAYER(22, 4)
      H(2,24)=H(22,4)
      LAYER(23,23)=LAYER( 3, 3)
      H(23,23)=H(3,3)
      LAYER(23,24)=LAYER( 3, 4)
      H(23,24)=H(3,4)
      LAYER(24,23)=LAYER( 4, 3)
      H(24,23)=H(4,3)
      LAYER(24,24)=LAYER( 4, 4)
      H(24,24)=H(4,4)
      DO 7 I=3,22
      EPS(1,I)=EPS(21,I)
      EPS(2,I)=EPS(22,I)
```

```
        EPS(23,I)=EPS(3,I)
        EPS(24,I)=EPS(4,I)
        EPS(I,1)=EPS(I,21)
        EPS(I,2)=EPS(I,22)
        EPS(I,23)=EPS(I,3)
        EPS(I,24)=EPS(I,4)
7       CONTINUE
C       CORNERS UPDATED
        EPS(1,1)=EPS(21,21)
        EPS(1,2)=EPS(21,22)
        EPS(2,1)=EPS(22,21)
        EPS(2,2)=EPS(22,22)
        EPS(23,1)=EPS(3,21)
        EPS(23,2)=EPS(3,22)
        EPS(24,1)=EPS(4,21)
        EPS(24,2)=EPS(4,22)
        EPS(1,23)=EPS(21,3)
        EPS(1,24)=EPS(21,4)
        EPS(2,23)=EPS(22,3)
        EPS(2,24)=EPS(22,4)
        EPS(23,23)=EPS(3,3)
        EPS(23,24)=EPS(3,4)
        EPS(24,23)=EPS(4,3)
        EPS(24,24)=EPS(4,4)
        RETURN
        END
        SUBROUTINE URNS(L,IRSIT,M)
        COMMON/BLK10/LL1,LL2,U1,MAXH,TA,TB
        DIMENSION IRSIT(300,3)
C          ALPHA DEPENDENT UPON THICKNESS OF B ON A OR HEIGHT
        AO=.1
        BO=.2
        ALPHA=AO*EXP(-BO*MAXH)
C       SCALE Y TO SITE INTERVAL
        DO 10 I=1,L
        Y1=URAN(0)
        Y2=URAN(0)
        IRSIT(I,1)=LL1+Y1*M
        IRSIT(I,2)=LL1+Y2*M
        IRSIT(I,3)=1
        IF(Y1.LT.ALPHA)IRSIT(I,3)=0
10      CONTINUE
        RETURN
        END
        SUBROUTINE UPDATE(RF,THETA,TH2,DC,HTS,JCODE)
        COMMON/BLK1/H,EPS(30,30),ITRAC(30,30,20)
        COMMON/BLK5/LAYER(30,30)
        COMMON/BLK10/LL1,LL2,U1,MAXH,TA,TB
        COMMON/BLK12/C
```

```
      INTEGER B(30,30),C(30,30)
      INTEGER H(30,30)
      DIMENSION DC(400),HTS(10)
      DIMENSION NEXT(400,2)
C     RF=ROUGHNESS FACTOR , RF=1 FOR FLAT SURFACE
C     THETA=COVERAGE, DC=DENSITY OF CLUSTERS(1,2,3,...,10)
      TB=0
      TA=0
      DO 80 II=3,22
      DO 81 JJ=3,22
         IJ=H(II,JJ)
      IF(ITRAC(II,JJ,IJ).EQ.0)TA=TA+1
      IF(ITRAC(II,JJ,IJ).EQ.1)TB=TB+1
81    CONTINUE
80    CONTINUE
      DO 5 I=1,400
5     DC(I)=0.
      CALL XYX
C     THETA =COVERAGE
      DO 10 II=1,10
10    HTS(II)=0.
      DO 50 I=3,22
      DO 50 J=3,22
      DO 51 IK=1,10
      IF(LAYER(I,J).GE.IK)HTS(IK)=HTS(IK)+1
51    CONTINUE
50    CONTINUE
      THETA=HTS(1)/400
      TH2=HTS(2)/400
      MAX=1
      DO 100 II=1,10
      IF(HTS(II).GE.20.)MAX=II
100   CONTINUE
      MAXH=MAX
      DO 8 I=1,24
      DO 8 J=1,24
      C(I,J)=1
      B(I,J)=0.
8     CONTINUE
      DO 9 I=1,24
      DO 9 J=1,24
      IF(LAYER(I,J).GE.MAX)B(I,J)=1.
9     CONTINUE
      SUM=0.
      DO 60 I=3,22
      DO 60 J=3,22
60    SUM=SUM+IABS(H(I,J)-H(I,J+1))
      RF=1+SUM/400.
      ILST=0
```

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```
         INXT=0
         ICT=0
         DO 20 I=3,22
         DO 20 J=3,22
         IF(B(I,J).EQ.0)GO TO 20
         LI=I
         LJ=J
         CALL CORRECT(LI,LJ)
25       ICT=ICT+1
         ILJ=LJ+1
         IF(B(LI,ILJ).EQ.0)GO TO 21
         IF(C(LI,ILJ).EQ.0)GO TO 21
         ILST=ILST+1
         NEXT(ILST,1)=LI
         NEXT(ILST,2)=ILJ
         CALL CORRECT(LI,ILJ)
21       ILJ=LJ-1
         IF(B(LI,ILJ).EQ.0)GO TO 22
         IF(C(LI,ILJ).EQ.0)GO TO 22
         ILST=ILST+1
         NEXT(ILST,1)=LI
         NEXT(ILST,2)=ILJ
         CALL CORRECT(LI,ILJ)
22       IF(JCODE.EQ.3)GO TO 24
         ILI=LI+1
         IF(B(ILI,LJ).EQ.0)GO TO 23
         IF(C(ILI,LJ).EQ.0)GO TO 23
         ILST=ILST+1
         NEXT(ILST,1)=ILI
         NEXT(ILST,2)=LJ
         CALL CORRECT(ILI,LJ )
23       ILI=LI-1
         IF(B(ILI,LJ).EQ.0)GO TO 74
         IF(C(ILI,LJ).EQ.0)GO TO 74
         ILST=ILST+1
         NEXT(ILST,1)=ILI
         NEXT(ILST,2)=LJ
         CALL CORRECT(ILI,LJ)
74          IF(JCODE.EQ.1)GO TO 24
         ILI=LI-1
         ILJ=LJ-1
         IF(B(ILI,ILJ).EQ.0)GO TO 76
         IF(C(ILI,ILJ).EQ.0)GO TO 76
         ILST=ILST+1
         NEXT(ILST,1)=ILI
         NEXT(ILST,2)=ILJ
         CALL    CORRECT(ILI,ILJ)
76          ILI=LI+1
         ILJ=LJ+1
```

```
        IF(B(ILI,ILJ).EQ.0)GO TO 24
        IF(C(ILI,ILJ).EQ.0)GO TO 24
        ILST=ILST+1
        NEXT(ILST,1)=ILI
        NEXT(ILST,2)=ILJ
        CALL CORRECT(ILI,ILJ)
24      B(LI,LJ)=0
        C(LI,LJ)=0
        IF(LI.GT.3)GO TO 30
        B(23,LJ)=0
        C(23,LJ)=0
30      IF(LI.LT.22)GO TO 31
        B(2,LJ)=0
        C(2,LJ)=0
31      IF(LJ.GT.3)GO TO 32
        B(LI,23)=0
        C(LI,23)=0
32      IF(LJ.LT.22)GO TO 33
        B(LI,2)=0
        C(LI,2)=0
33      CONTINUE
        IF(INXT.EQ.ILST)GO TO 26
        INXT=INXT+1
        LI=NEXT(INXT,1)
        LJ=NEXT(INXT,2)
        IF(LI.LT.3)LI=22
        IF(LI.GT.22)LI=3
        IF(LJ.LT.3)LJ=22
        IF(LJ.GT.22)LJ=3
        GO TO 25
26      ILST=0
        INXT=0
        DC(ICT)=DC(ICT)+1
        ICT=0
20      CONTINUE
        RETURN
        END
        SUBROUTINE CORRECT(II,JJ)
        COMMON/BLK5/LAYER(30,30)
        COMMON/BLK12/C
        INTEGER C(30,30)
        C(II,JJ)=0
        IF(JJ.EQ.2)GO TO 2
        IF(JJ.EQ.3)GO TO 3
        IF(JJ.EQ.22)GO TO 22
        IF(JJ.EQ.23)GO TO 23
        IF(II.EQ.2)GO TO 32
        IF(II.EQ.3)GO TO 33
        IF(II.EQ.22)GO TO 34
```

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```
            IF(II.EQ.23)GO TO 35
            RETURN
2           C(II,22)=0
17          IF(II.EQ.2)C(22,JJ)=0
            IF(II.EQ.3)C(23,JJ)=0
            IF(II.EQ.22)C(2,JJ)=0
            IF(II.EQ.23)C(3,JJ)=0
            GO TO 24
3           C(II,23)=0
            GO TO 17
22          C(II,2)=0
            GO TO 17
23          C(II,3)=0
            GO TO 17
32          C(22,JJ)=0
18          IF(JJ.EQ.2)C(II,22)=0
            IF(JJ.EQ.3)C(II,23)=0
            IF(JJ.EQ.22)C(II,2)=0
            IF(JJ.EQ.23)C(II,3)=0
            GO TO 24
33          C(23,JJ)=0
            GO TO 18
34          C(2,JJ)=0
            GO TO 18
35          C(3,JJ)=0
            GO TO 18
24          CONTINUE
            IF((II.EQ.3).AND.(JJ.EQ.3))C(23,23)=0
            IF((II.EQ.3).AND.(JJ.EQ.22))C(23,2)=0
            IF((II.EQ.22).AND.(JJ.EQ.3))C(2,23)=0
            IF((II.EQ.22).AND.(JJ.EQ.22))C(2,2)=0
            RETURN
            END
            SUBROUTINE MIXUP(IS,NS)
            DIMENSION L(401),IS(401)
            IC=1
            IF(NS.EQ.1)GO TO 100
            DO 50 KS=1,NS
50          L(KS)=KS
            M=NS
500         IF(M.EQ.2)GO TO 102
            R=RANF(0)
            I=1+R*M
            IF(   I.EQ.1)GO TO 51
            IF(I.EQ.M)GO TO 52
            IS(IC)=L(I)
            L(I)=L(M)
            M=M-1
            IC=IC+1
```

```
            GO TO 500
   51       IS(IC)=L(1)
            L(1)=L(M)
            M=M-1
            IC=IC+1
            GO TO 500
   52       IS(IC)=L(M)
            M=M-1
            IC=IC+1
            GO TO 500
  100       IS(1)=1
            RETURN
  102       R=RANF(0)
            I=1+R*M
            IF(I.EQ.1)GO TO 101
            IS(IC)=L(2)
            IS(IC+1)=L(1)
            RETURN
  101       IS(IC)=L(1)
            IS(IC+1)=L(2)
            RETURN
            END
```
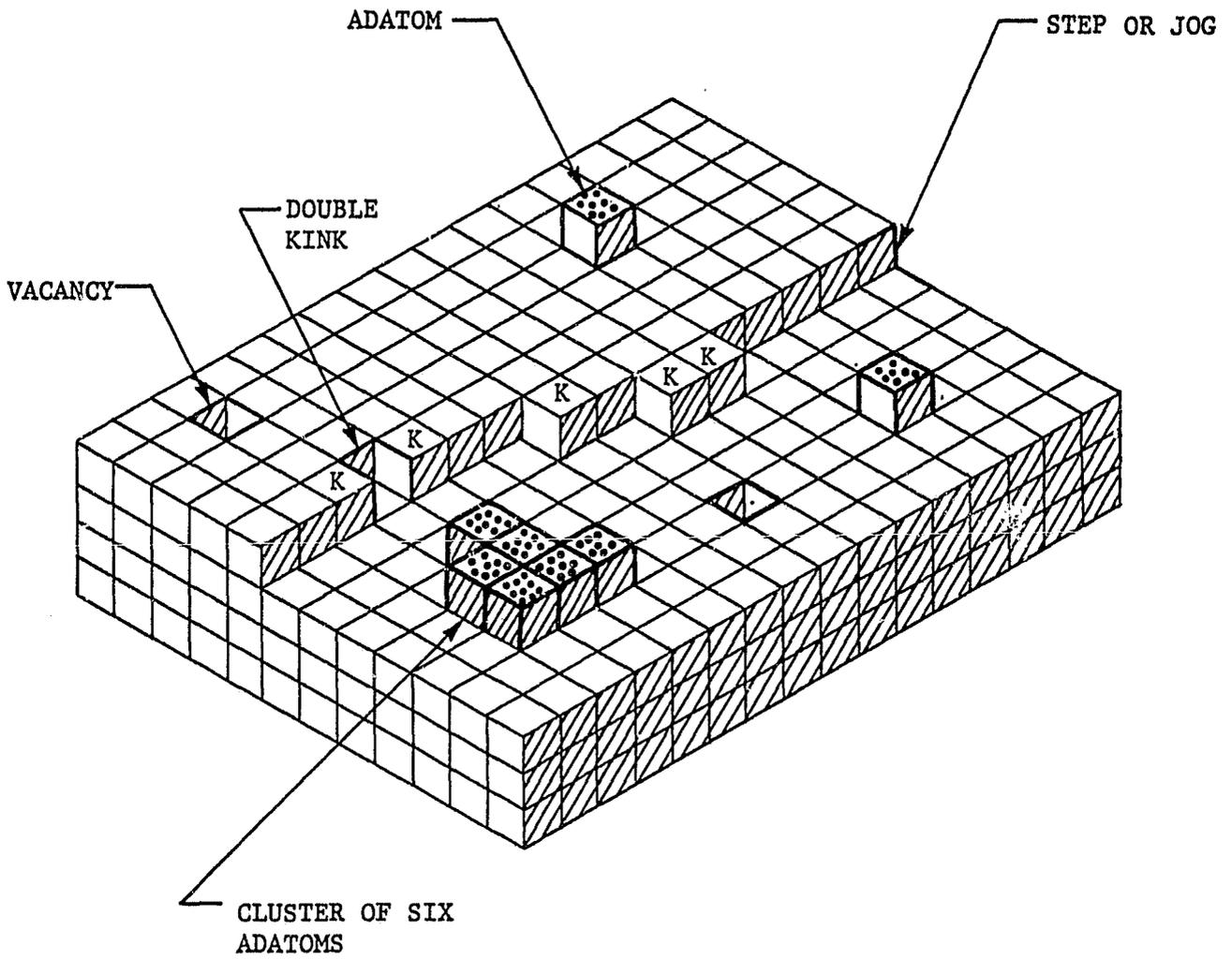
Figure 1.   SOS model for crystal growth.
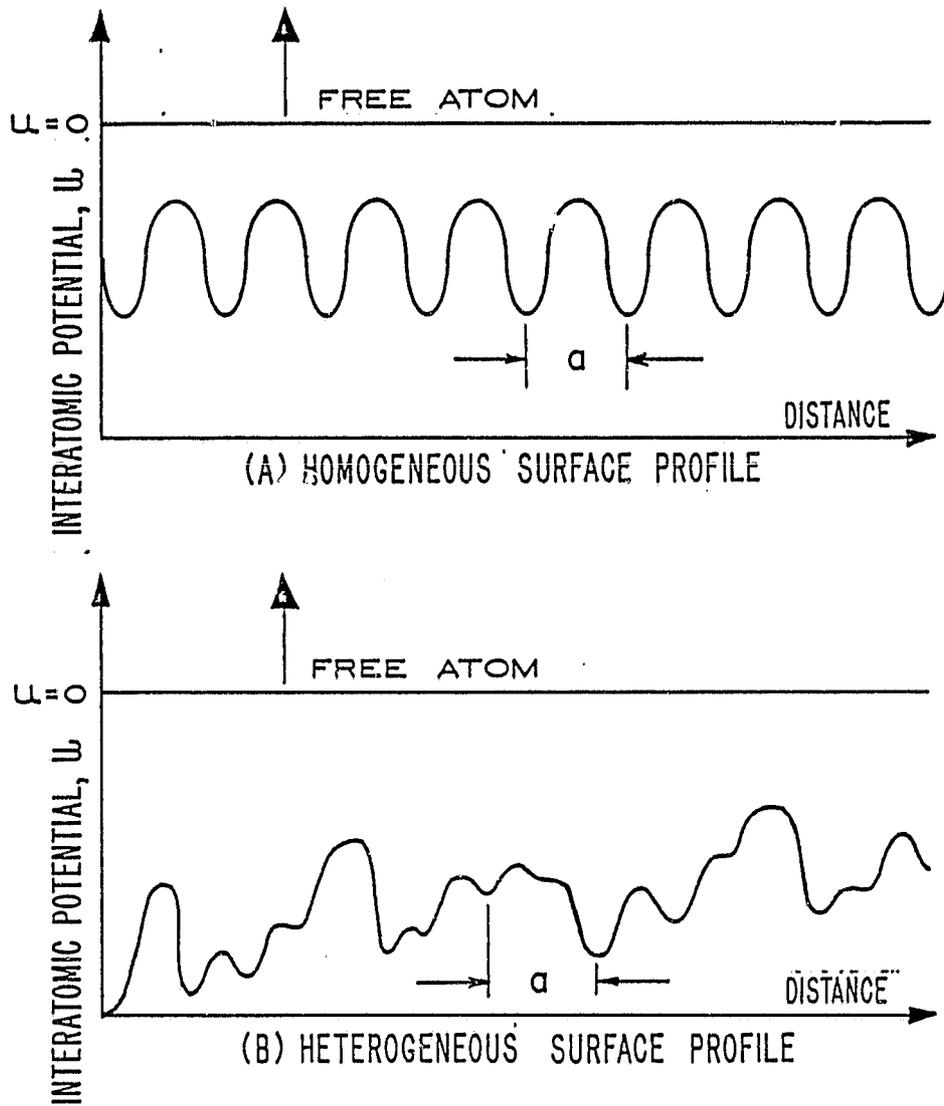
Figure 2. Profile of surface potentials (a) uniform homogenous surface
(b) vacancies, dislocations, kinks, jogs and impurities disturb
the surface potential.

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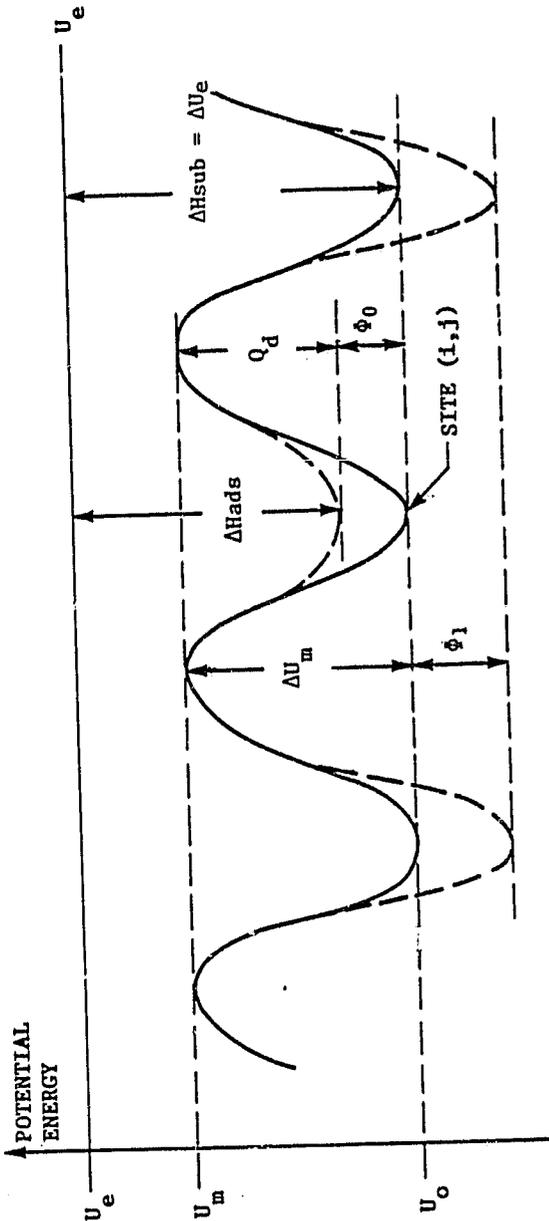
$\Delta Hads$ = HEAT OF ADSORPTION FOR SINGLE ADATOM

$\Delta Hsub$ = HEAT OF SUBLIMATION

U_e = EVAPORATION BARRIER

U_m = MIGRATION BARRIER

U_0 = $-\Delta Hevap$ = NOMINAL VALUE FOR POTENTIAL UNIFORM SURFACE

Φ_0 = $\Delta Hevap - \Delta Hads$ = POTENTIAL CHANGE DUE TO ADDITION OF ADATOM AT SITE (i,j)

Φ_1 = NEAREST NEIGHBOR POTENTIAL CHANGE

Φ_2 = SECOND NEAREST NEIGHBOR POTENTIAL CHANGE

Q_d = DIFFUSION ACTIVATION ENERGY

Figure 3. Potentials for a uniform flat surface (solid line) and potential after an adatom has been added to site (i,j) (dashed line).
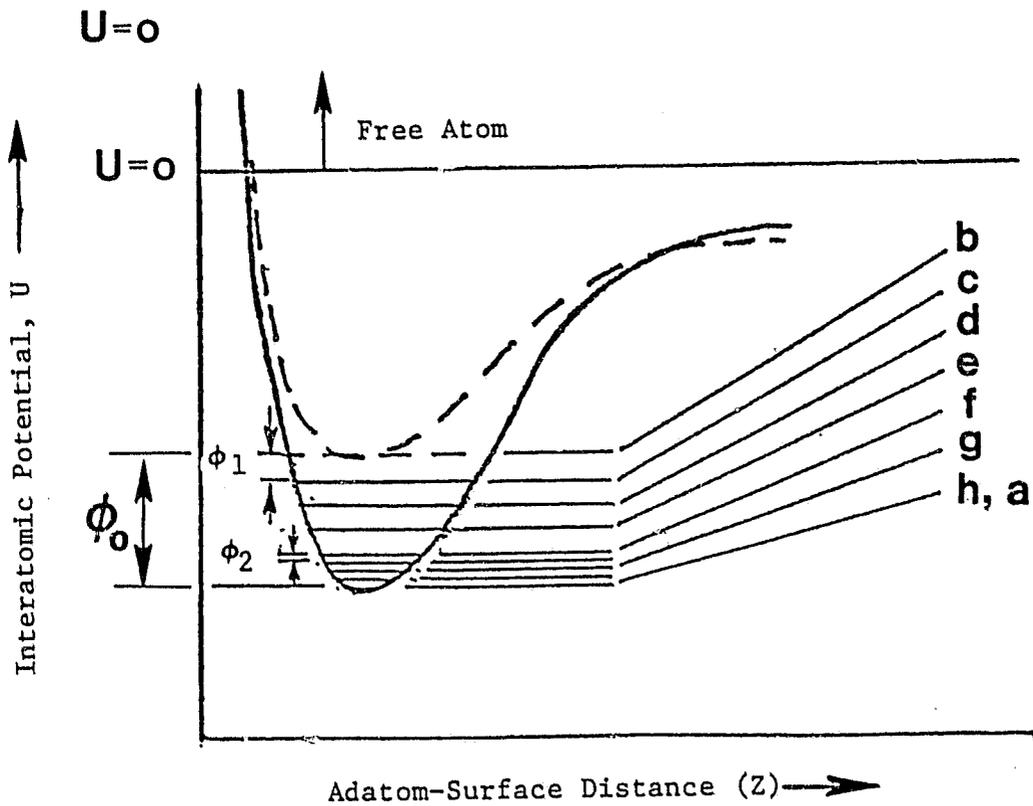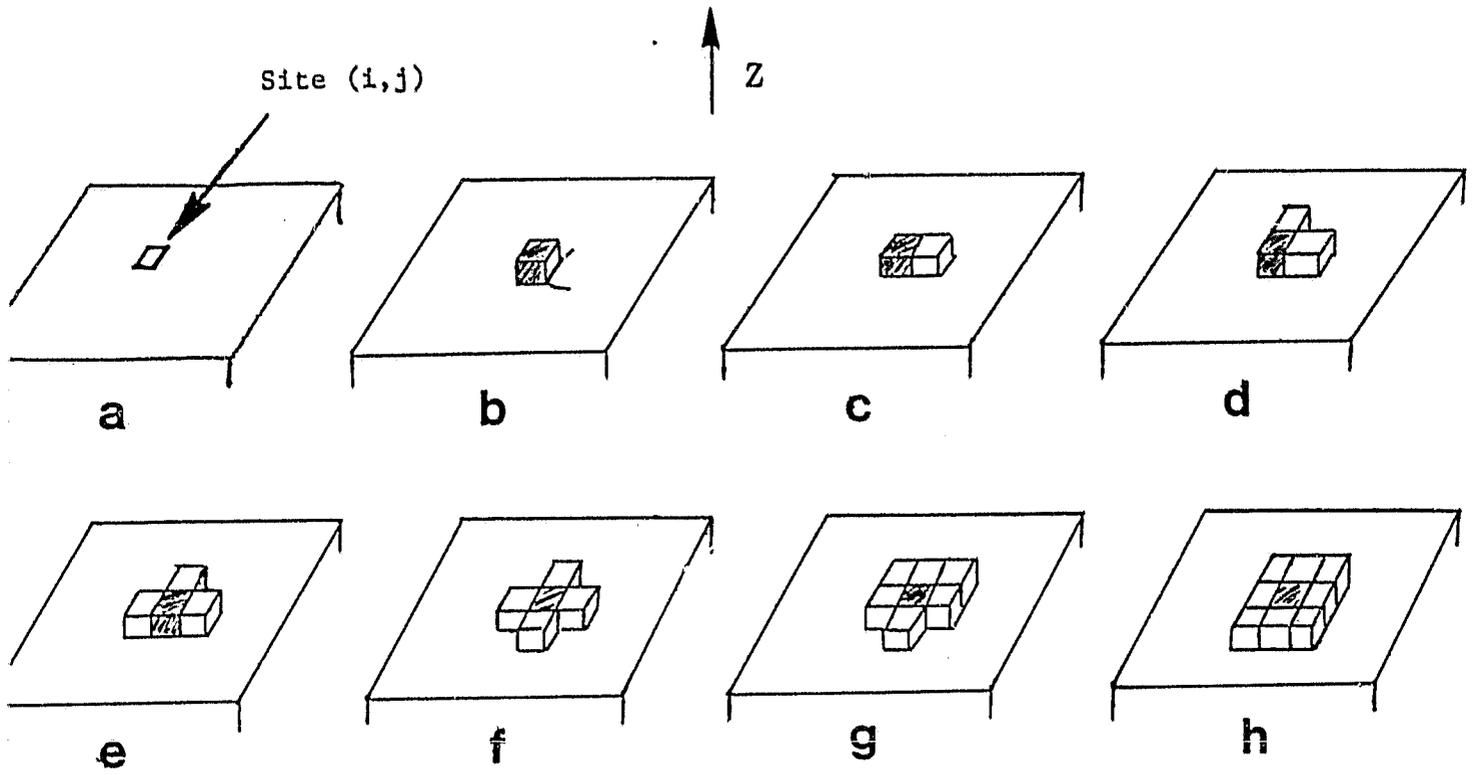
Figure 4.   Potential variation at an arbitrary site (i,j).

[001]

[010]

[100]

X

MNEMONIC MASK

ϕ_2

ϕ_1 ϕ_1

ϕ_2 ϕ_0 ϕ_2

ϕ_1 ϕ_1

ϕ_2

$-\phi_2$	$-\phi_1$	$-\phi_2$
$-\phi_1$	ϕ_0	$-\phi_1$
$-\phi_2$	$-\phi_1$	$-\phi_2$

MNEMONIC MASK

ϕ_2

ϕ_2 ϕ_1 ϕ_1 ϕ_2

ϕ_1 ϕ_0 ϕ_1

ϕ_2 ϕ_1 ϕ_1 ϕ_2

ϕ_2

$$-\phi_2$$

$-\phi_2$	$-\phi_1$	$-\phi_1$	$-\phi_2$	
	$-\phi_1$	ϕ_0	$-\phi_1$	
	$-\phi_2$	$-\phi_1$	$-\phi_1$	$-\phi_2$

$$-\phi_2$$

MNEMONIC MASK

ϕ_3 ϕ_2 ϕ_3

ϕ_1 ϕ_0 ϕ_1

ϕ_3 ϕ_2 ϕ_3
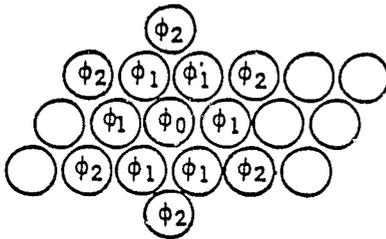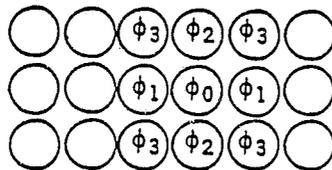
$-\phi_3$	$-\phi_2$	$-\phi_3$
$-\phi_1$	ϕ_0	$-\phi_1$
$-\phi_3$	$-\phi_2$	$-\phi_3$

Figure 5. FCC model and potential changes associated with different crystal orientations.

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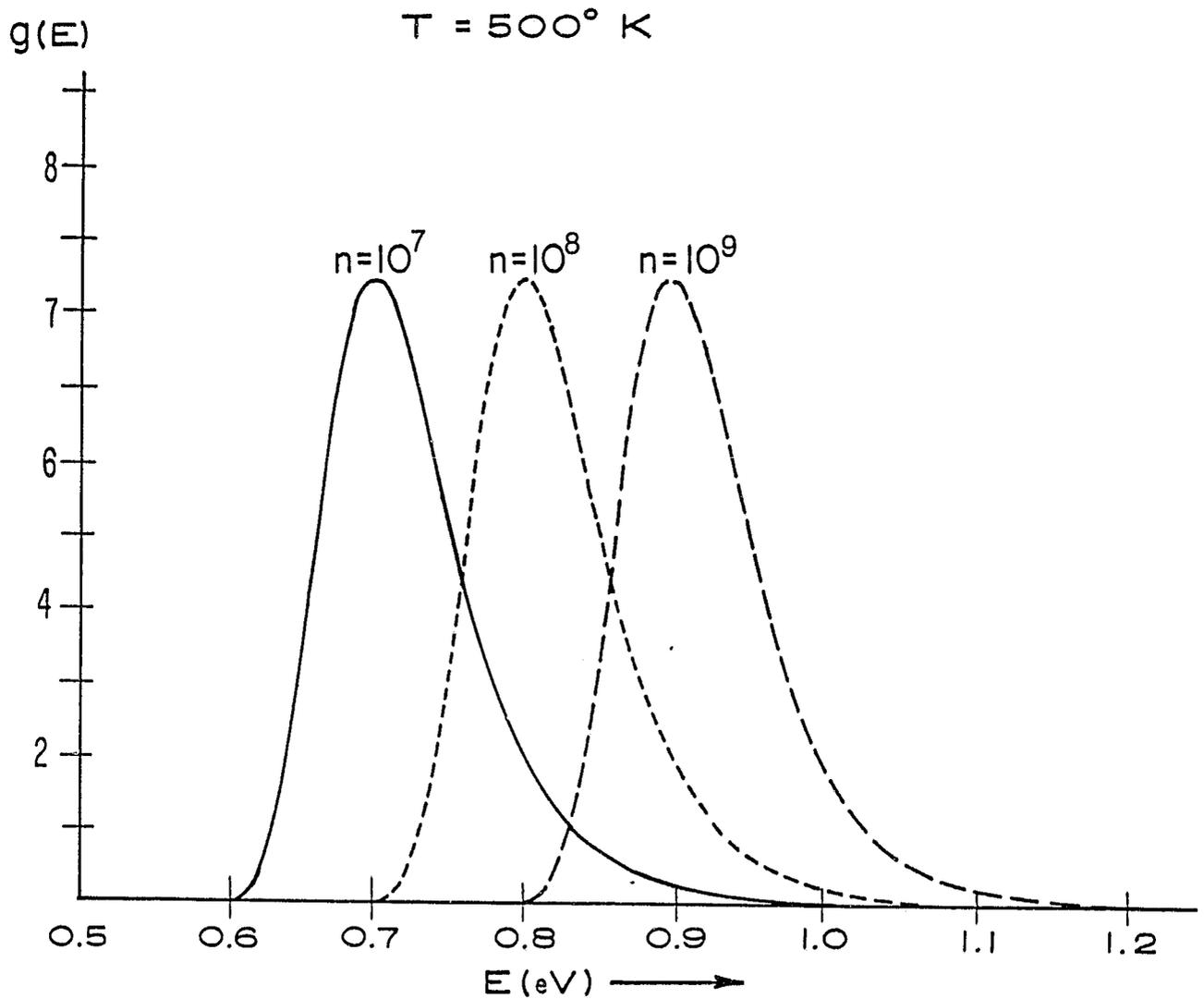
Figure 6. Probability density for the Boltzmann ordered statistic $E_{(n)}$ with $n = 10^7$, 10^8, 10^9 and $T = 500$ K.

Read value of parameters

Initialization of substrate geometry and potentials

Update time counter

Analysis of deposition rate and scan time → No deposition Scan surface

Impingement of L adatoms
Uniform distribution: Generate L random sites and deposit adatoms at these sites — update potentials

Scan surface:
Do for all surface sites (i,j)

Boltzmann distribution-ordered statistic
Generate random energy $E(i,j)$

Test potential at site (i,j)
$U = U_0(i,j) + E(i,j)$
If $U < U_m$ then localization
If $U > U_e$ then evaporation
If $U_i \leqslant U < U_e$ then incorporation
If $U_m \leqslant U < U_i$ then surface diffusion

Localization:
Leave adatom at site (i,j)

Migration, evaporation, incorporation
save all sites in an array

Continue

Randomize order of saved array

Do for all entries of saved array

If evaporation or incorporation remove adatom from surface and update potentials

If migration: random walk to neighbor site and make potential changes

Continue

Calculate: various "measures" of crystal growth

Yes ← Again → No Stop

Figure 7. Flowchart for the Monte Carlo SOS computer simulation of thin film growth.

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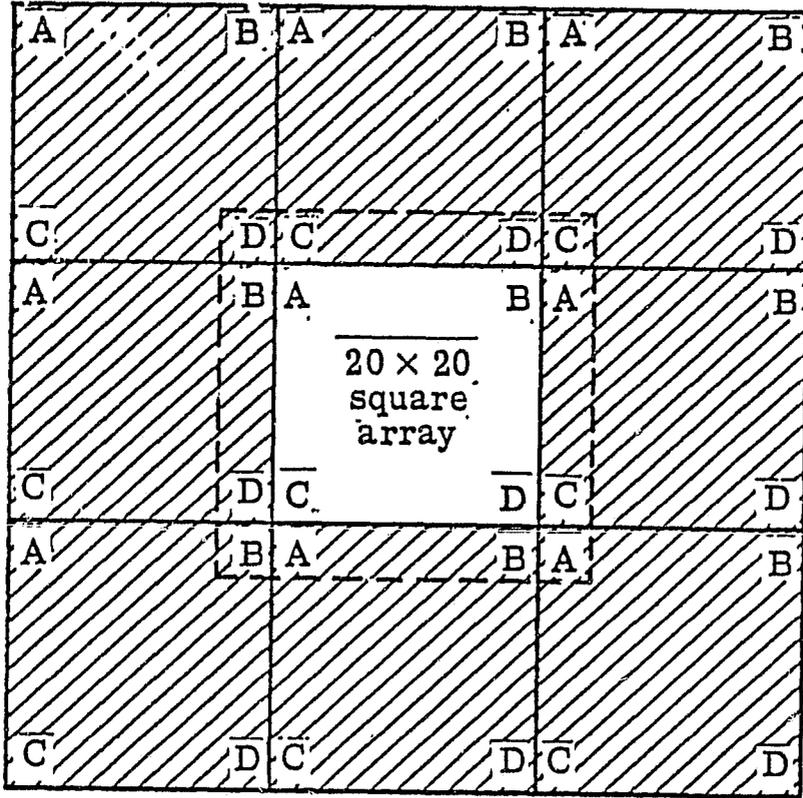
Figure 8.   A 20 × 20 square array with periodic extension.
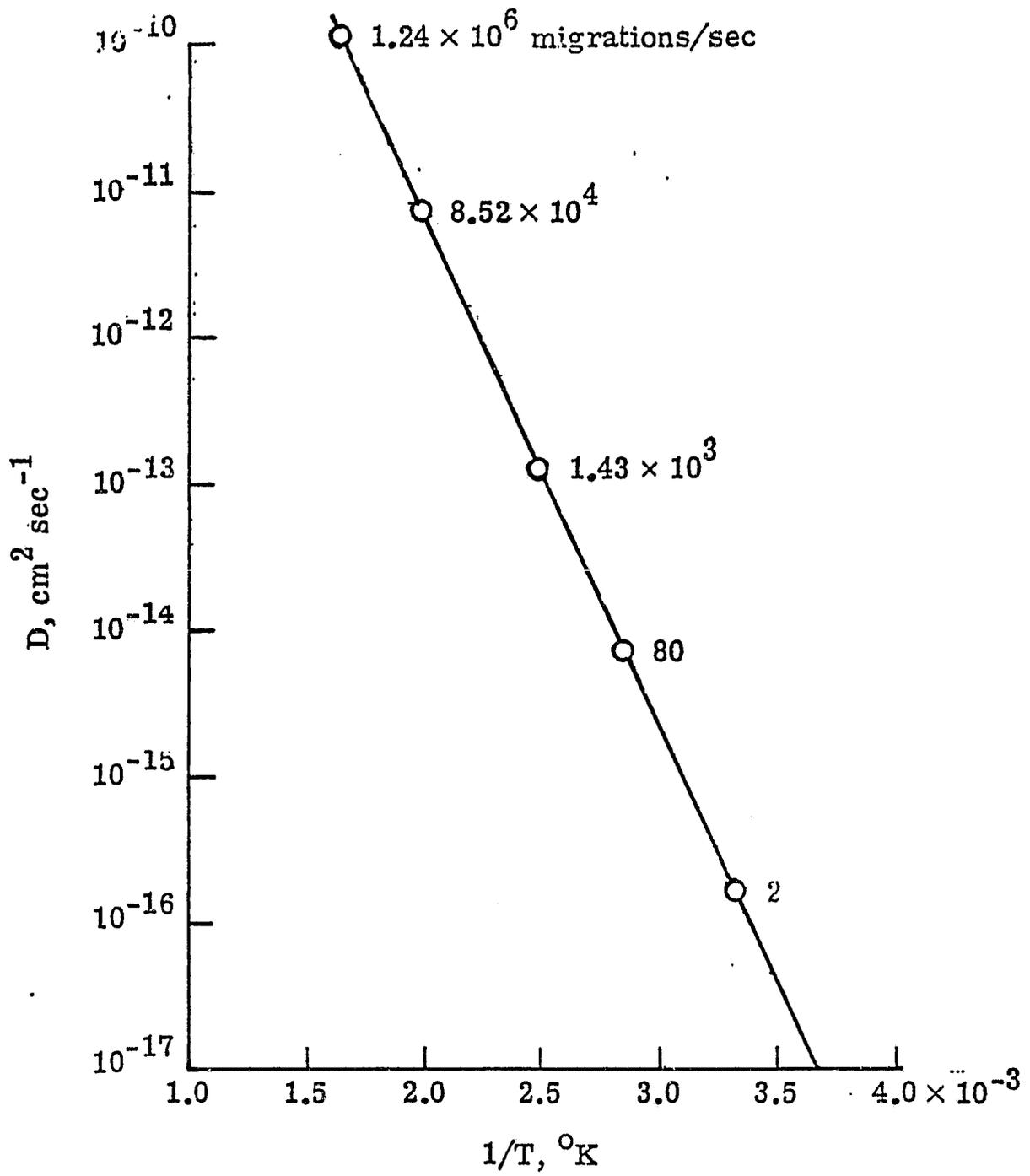
Figure 9. Diffusion coefficient vs. inverse temperature.
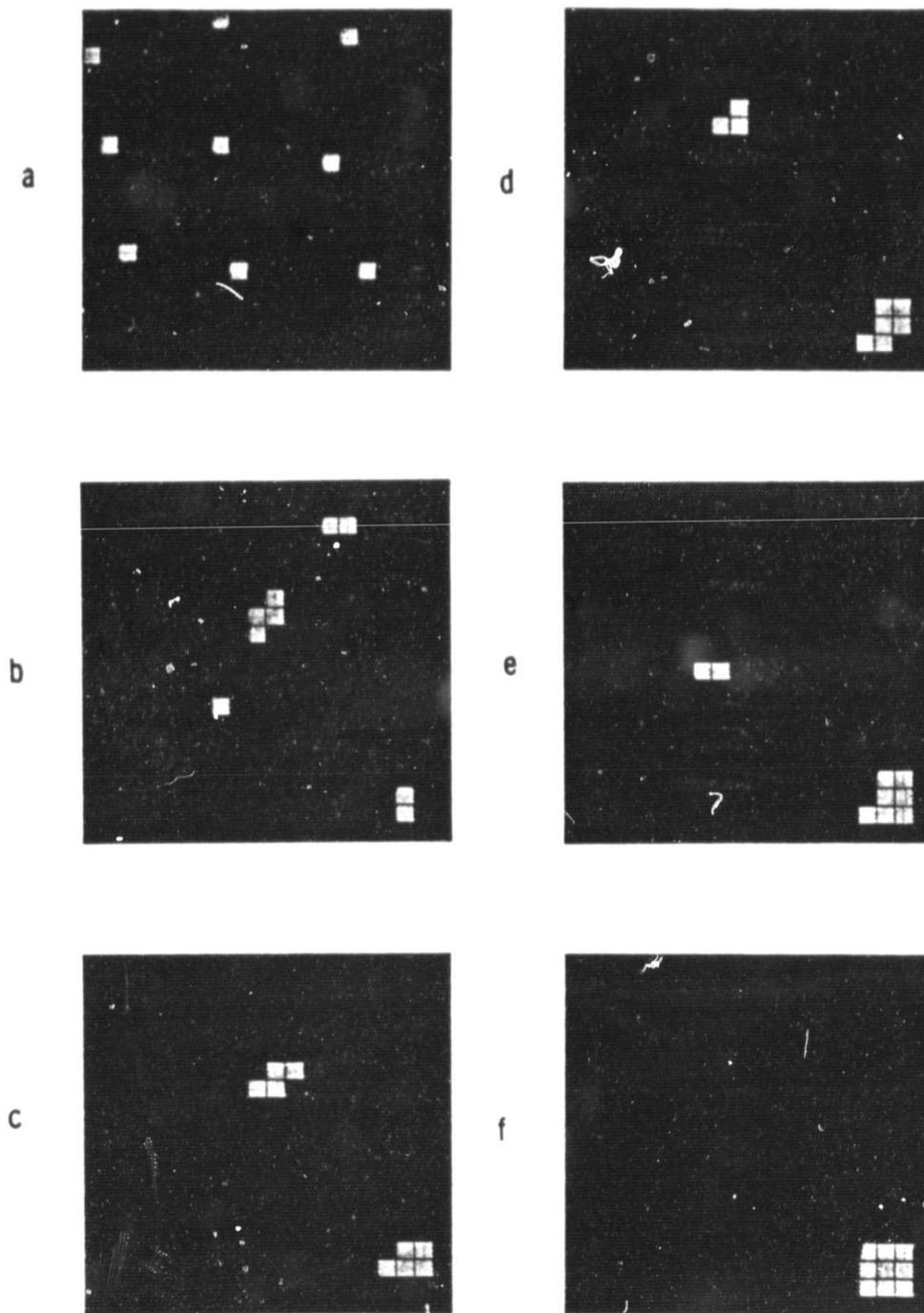
Figure 10. Clustering of dispersed adatoms on a uniform surface:
T = 600 K, (a) t = 0, (b) t = 0.1 s, (c) t = 0.3 s,
(d) t = 0.5 s, (e) t = 0.7 s, (f) t = 1.0 s.

1st layer

-3.87	-5	-3.87
-5	-6	-5
-3.87	-5	-3.87

2nd layer

-3.87	-3.87	-3.87
-3.87	-5	-3.87
-3.87	-3.87	-3.87

Figure 11. Trap potential variation for first and second layer.
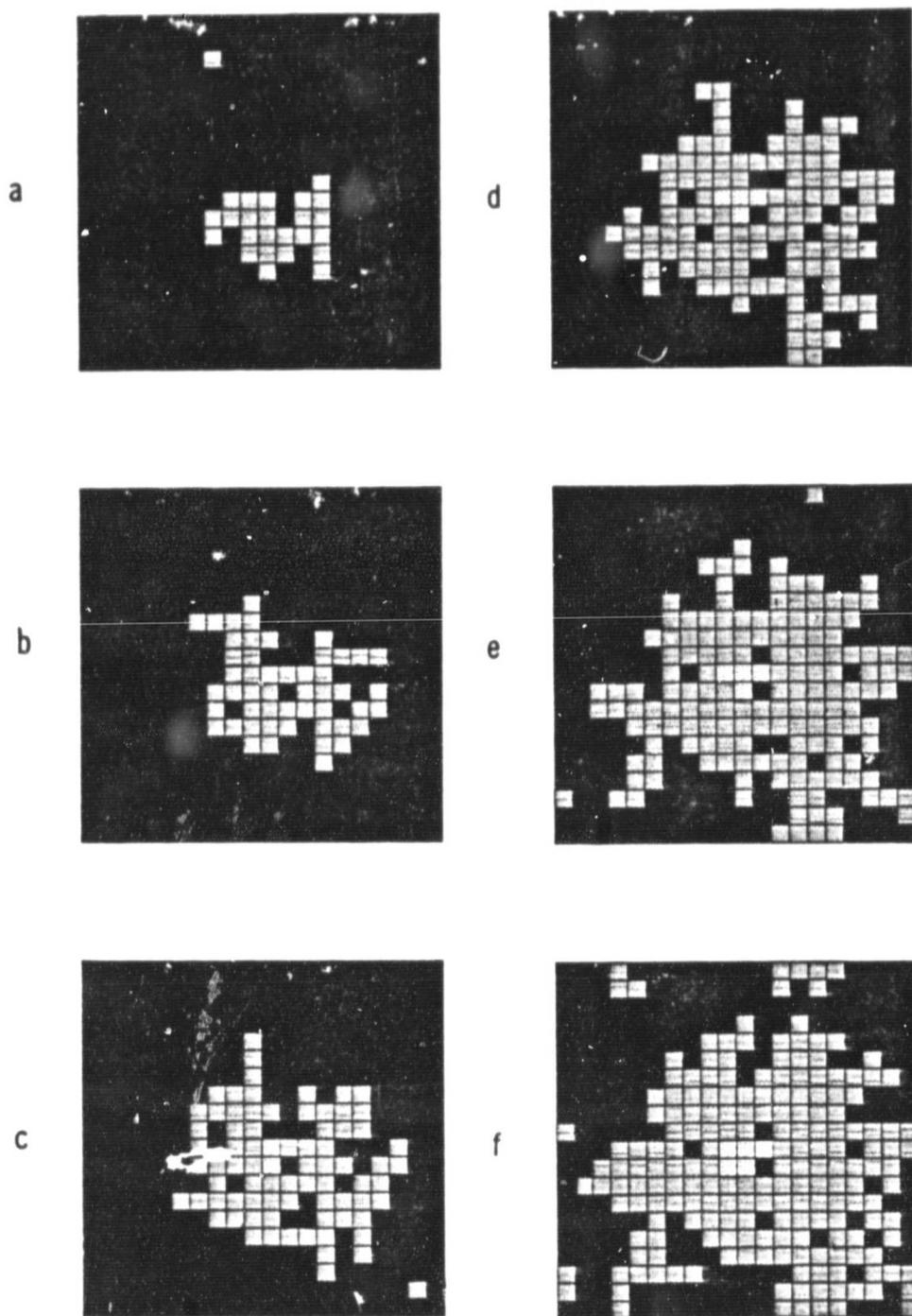
Figure 12   Growth around a trap: T = 550 K, (a) t = 0.5 s, (b) t = 0.8 s, (c) t = 1.1 s, (d) t = 1.4 s (e) t = 1.7 s, (f) t = 2.0 s, R_d = 0.2778 nm/sec.
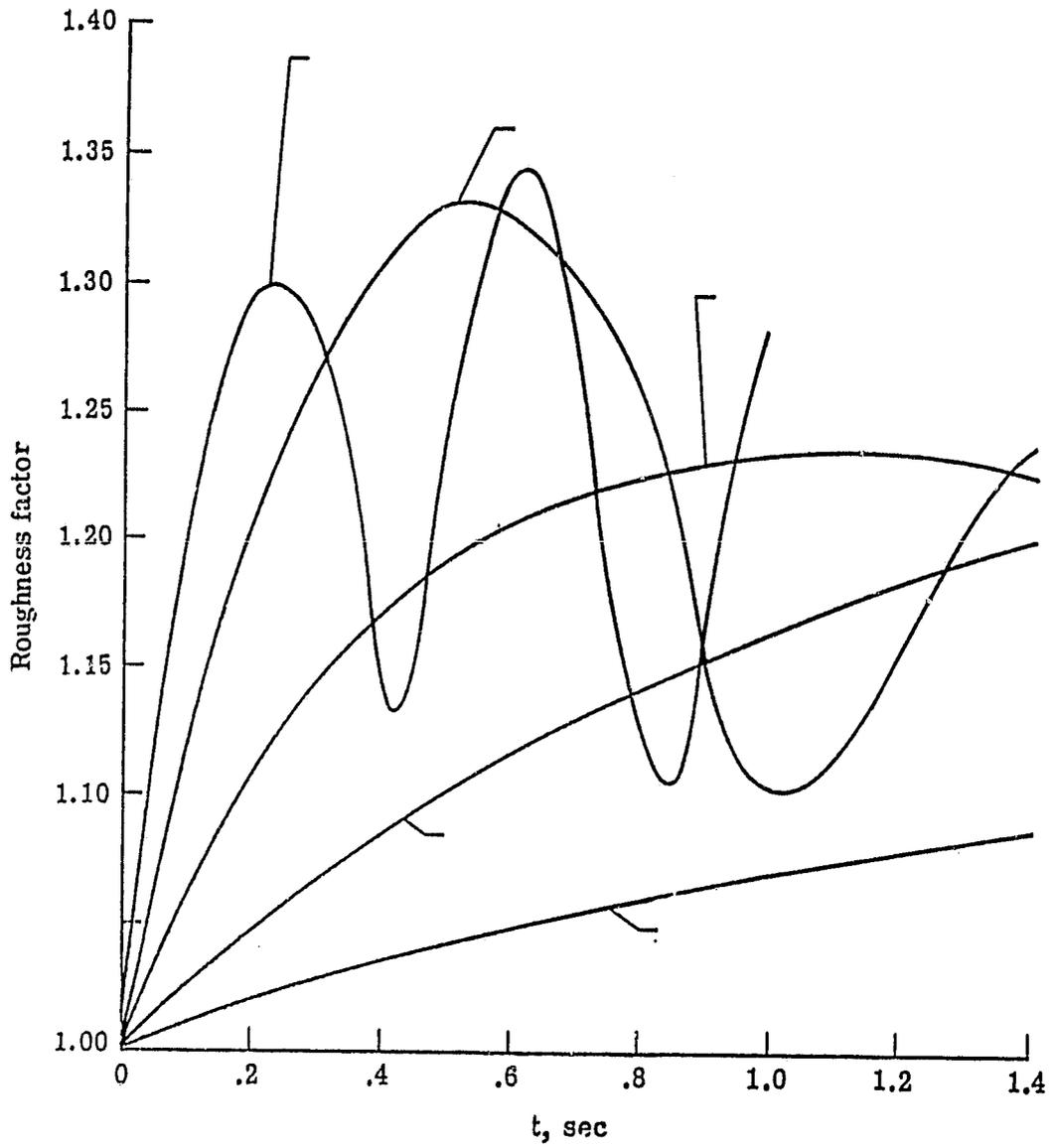
Figure 13. Surface roughness factor for T = 500 K and several deposition rates.
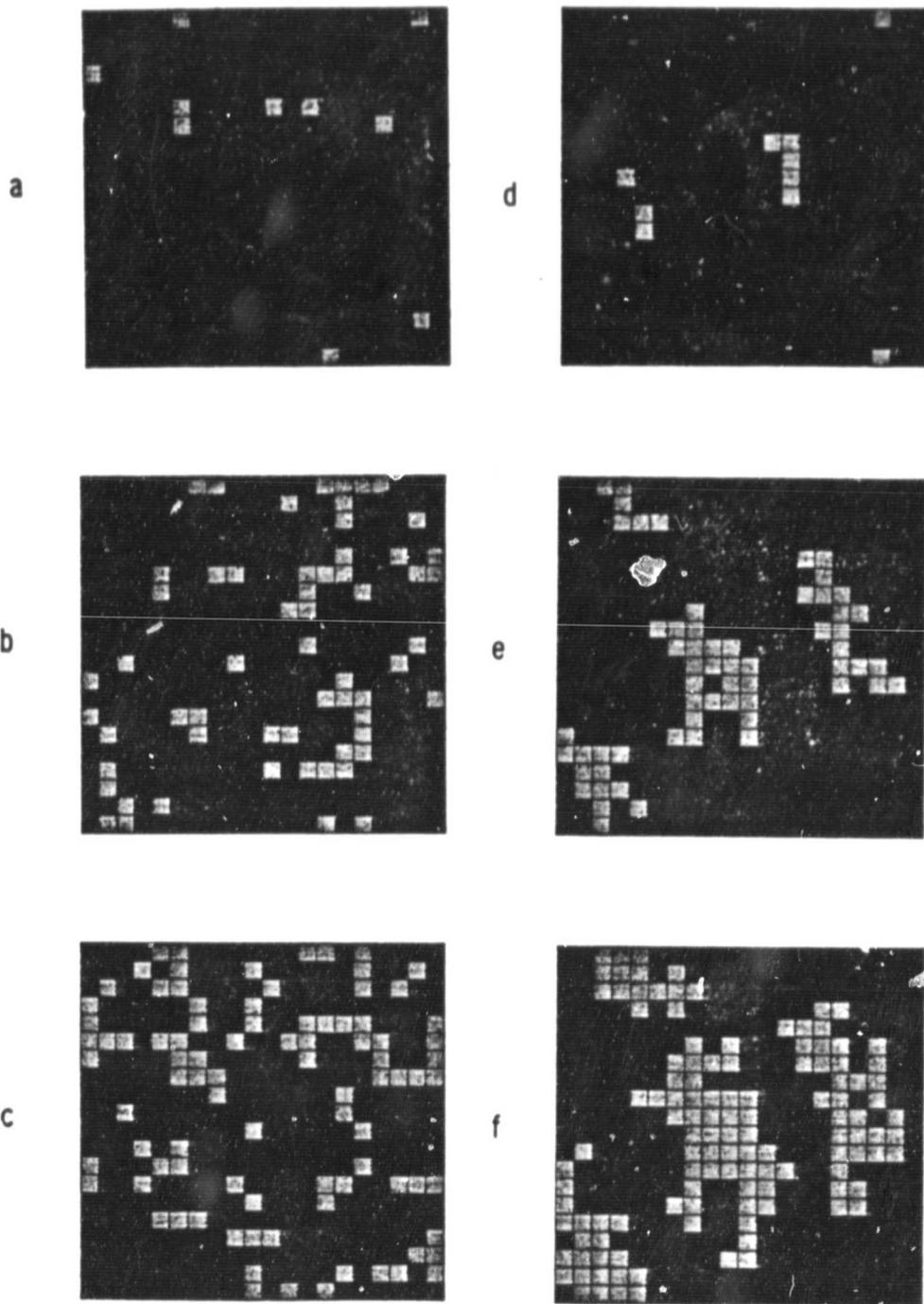
Figure 14. Thin film growth for R_d = 0.2778 nm/sec for two different temperatures, T = 300 K, (a) t = 0.5 s, (b) t = 3.0 s, (c) t = 6.0 s, T = 400 K, (d) t = 0.5 s, (e) t = 3.0 s (f) t = 6.0 s.

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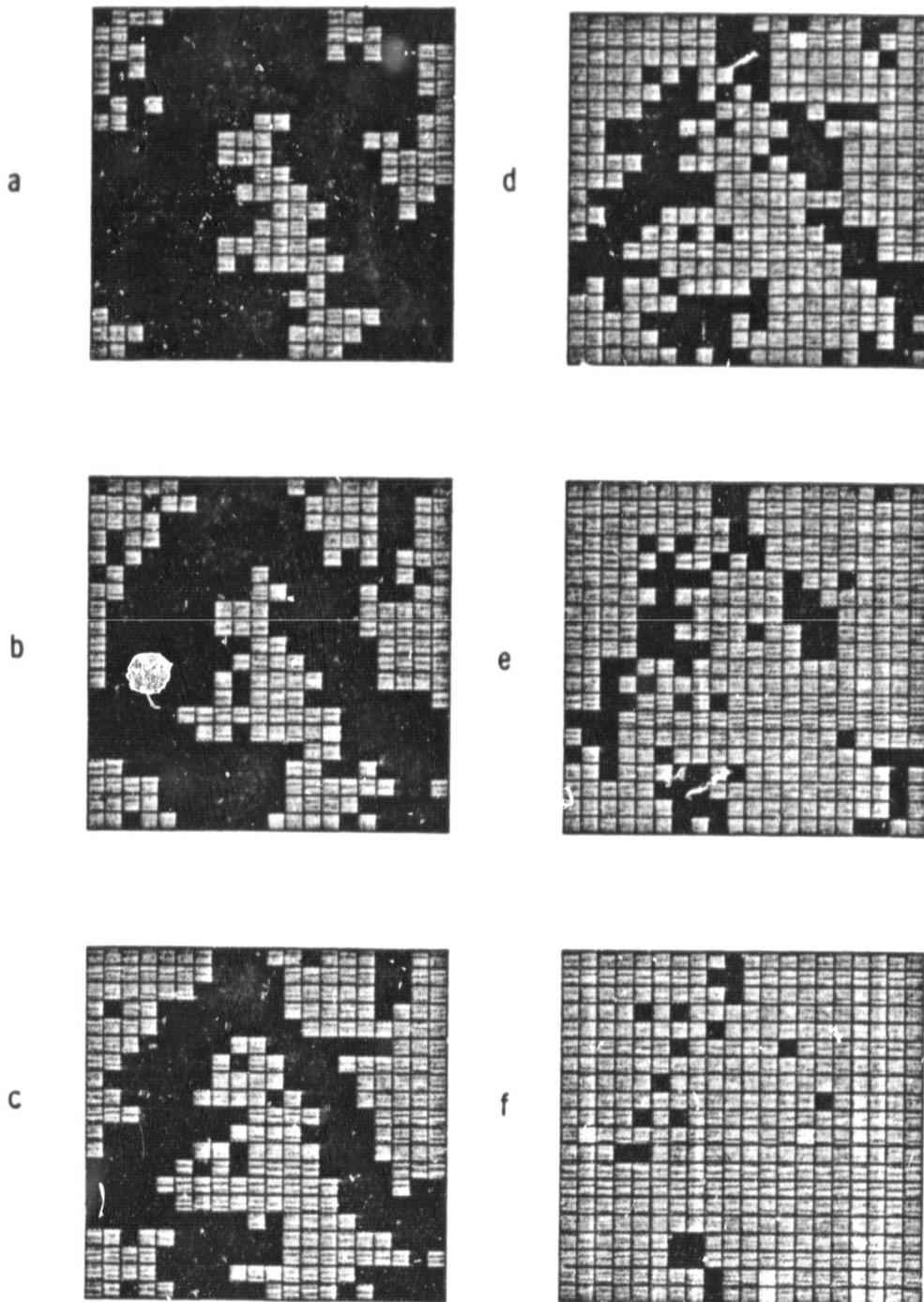
Figure 15. Thin film growth for R_d = 0.2778 nm/sec, T = 500 K, (a) t = 0.5 s, (b) t = 0.8 s, (c) t = 1.1 s, (d) t = 1.4 s, (e) t = 1.7 s, (f) t = 2.0 s.
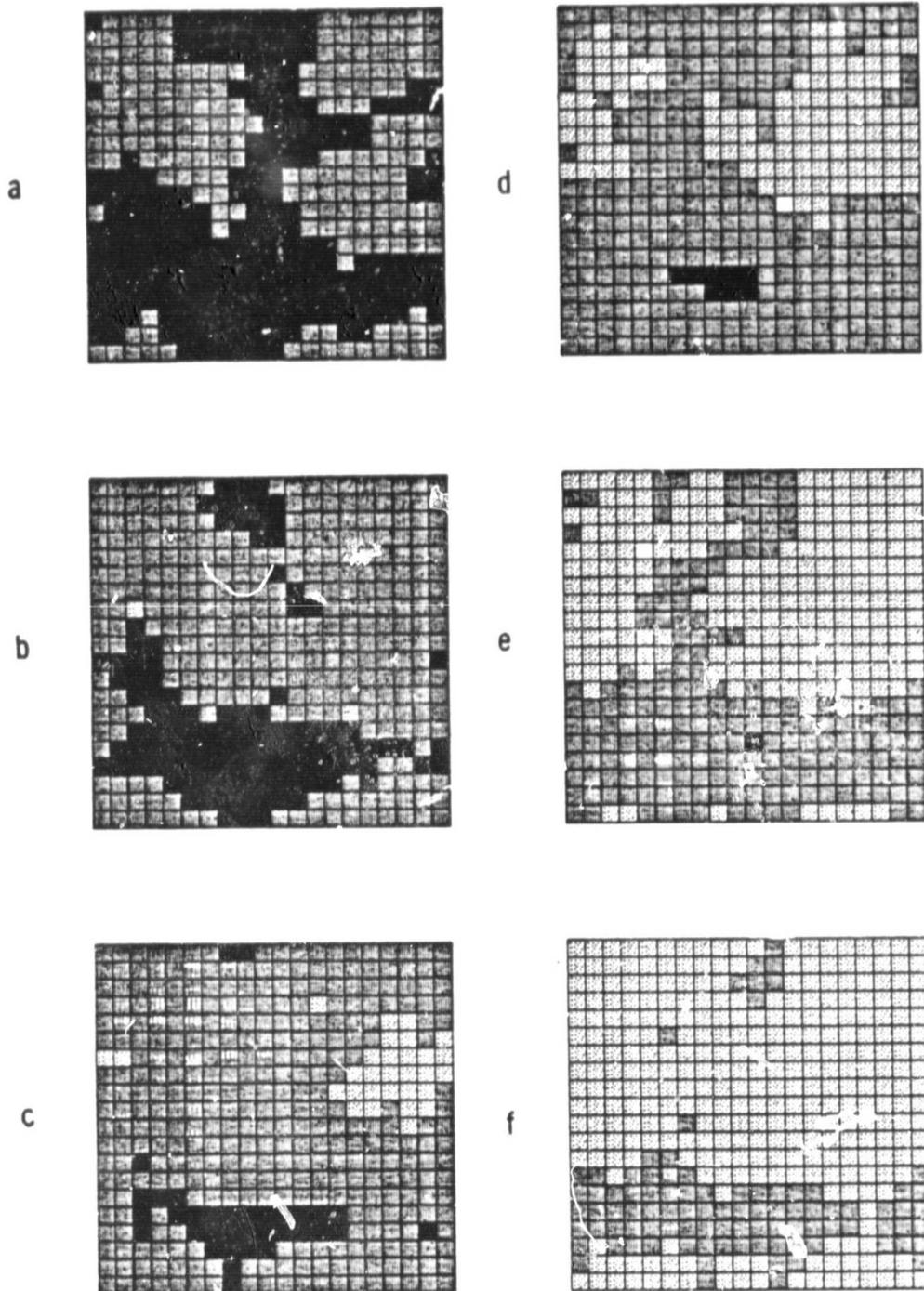
Figure 16. Thin film growth for R_d = 0.5556 nm/sec, T = 600 K,
(a) t = 0.5 s, (b) t = 0.8 s. (c) t = 1.1 s, (d) t =
1.4 s, (e) t = 1.7 s, (f) t = 2.0 s.
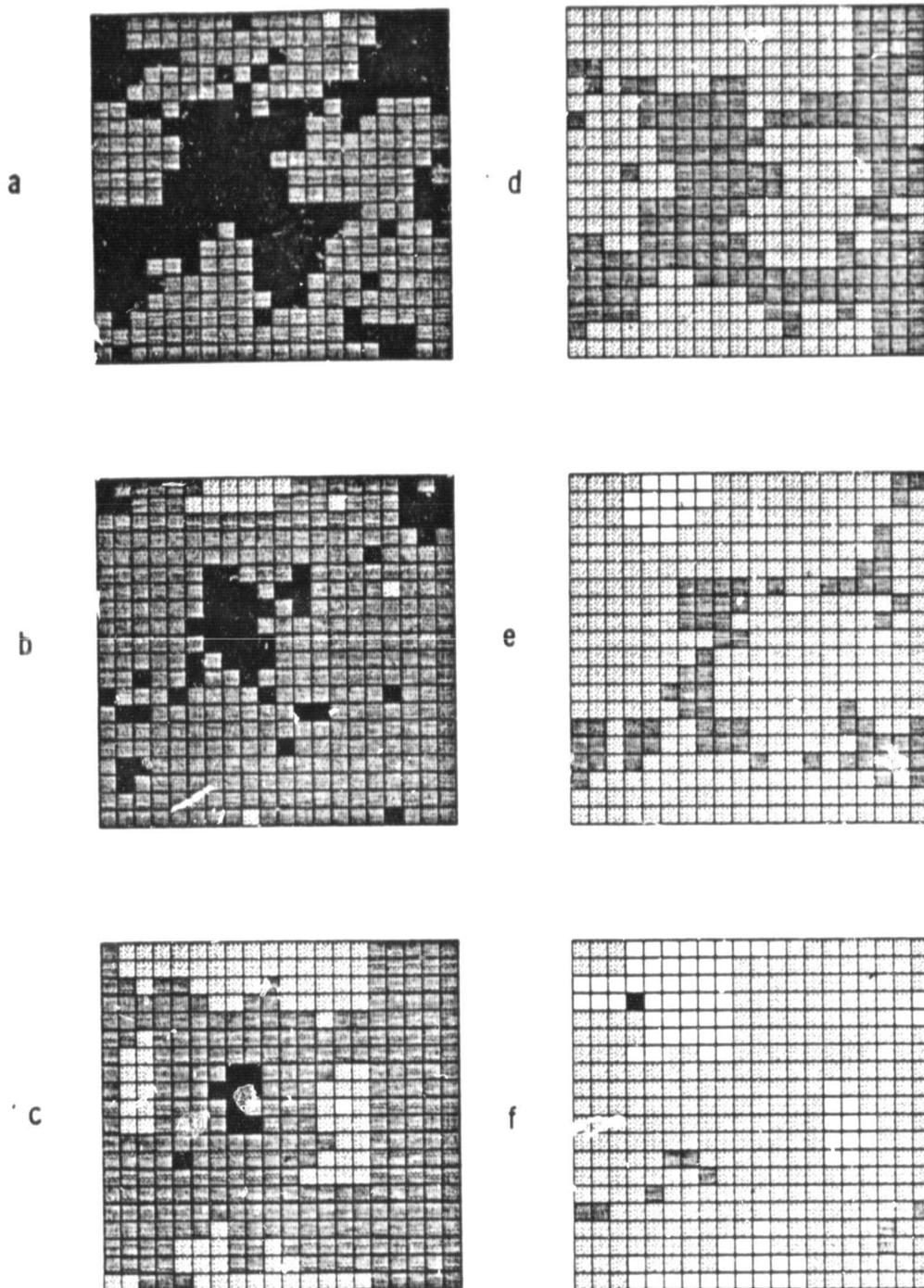
Figure 17. Thin film growth for R_i = 1.389 nm/sec, T = 600 K,
(a) t = 0.25 s, (b) t = 0.4 s, (c) t = 0.55 s, (d) t =
0.7 s, (e) t = 0.85 s (f) t = 1.0 s.
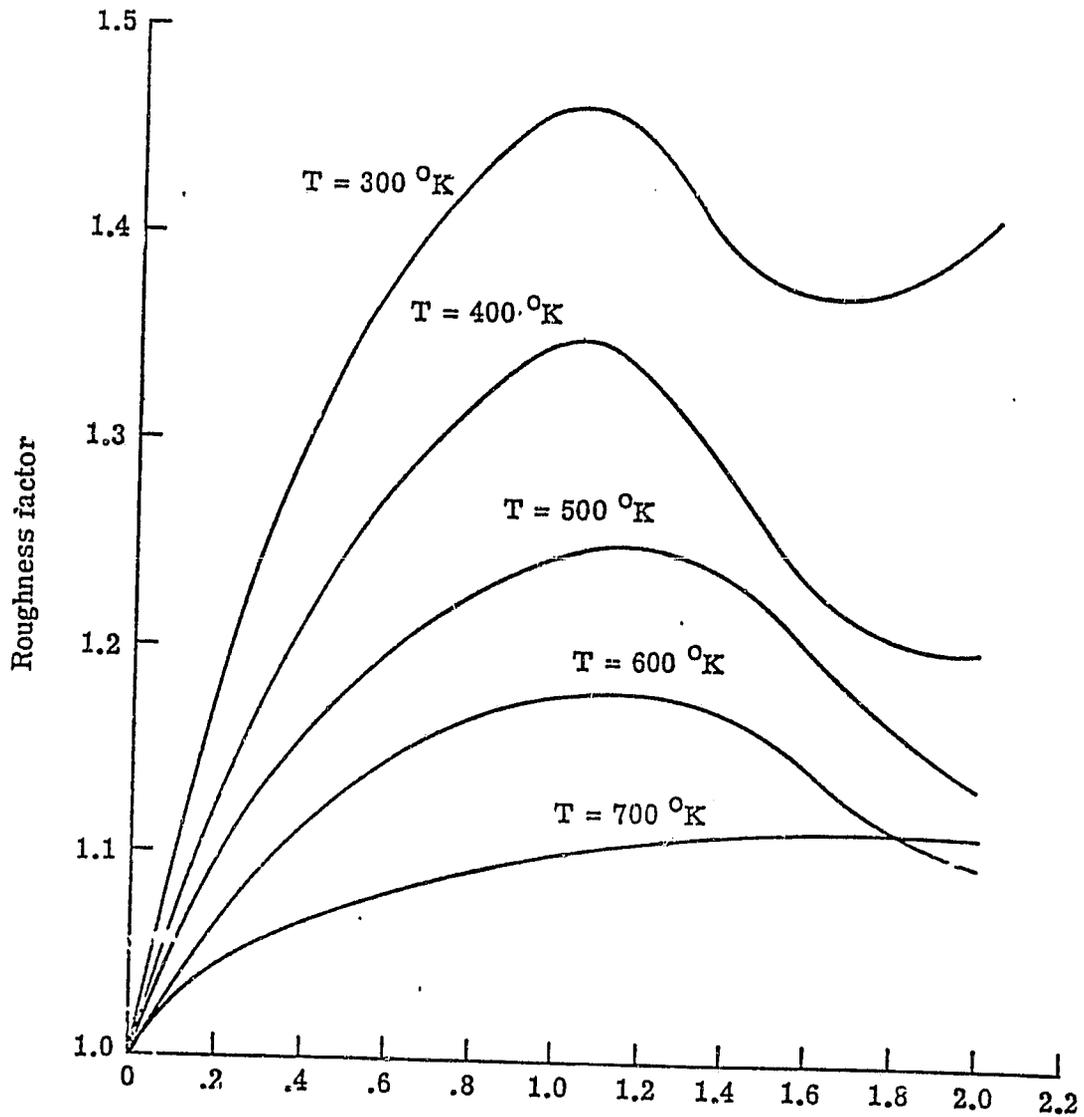
Figure 18. Surface roughness factor for $R_d = 0.2778$ nm/sec and various
temperatures.
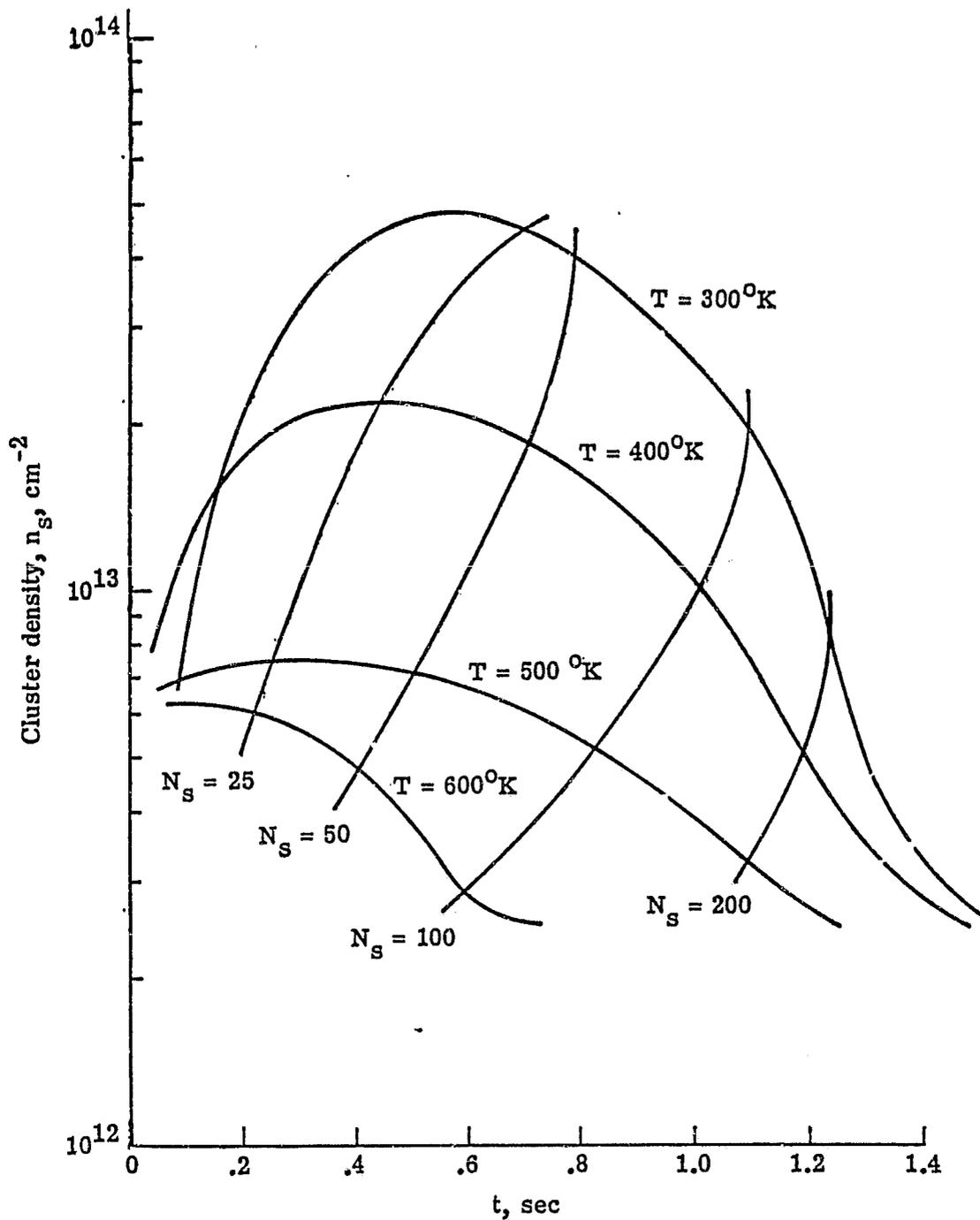
Figure 19. Nucleation density n_s as a function of time with constant cluster curves for 25, 50, 100 and 200 atoms. The decrease in n_s corresponds to growth coalescence.
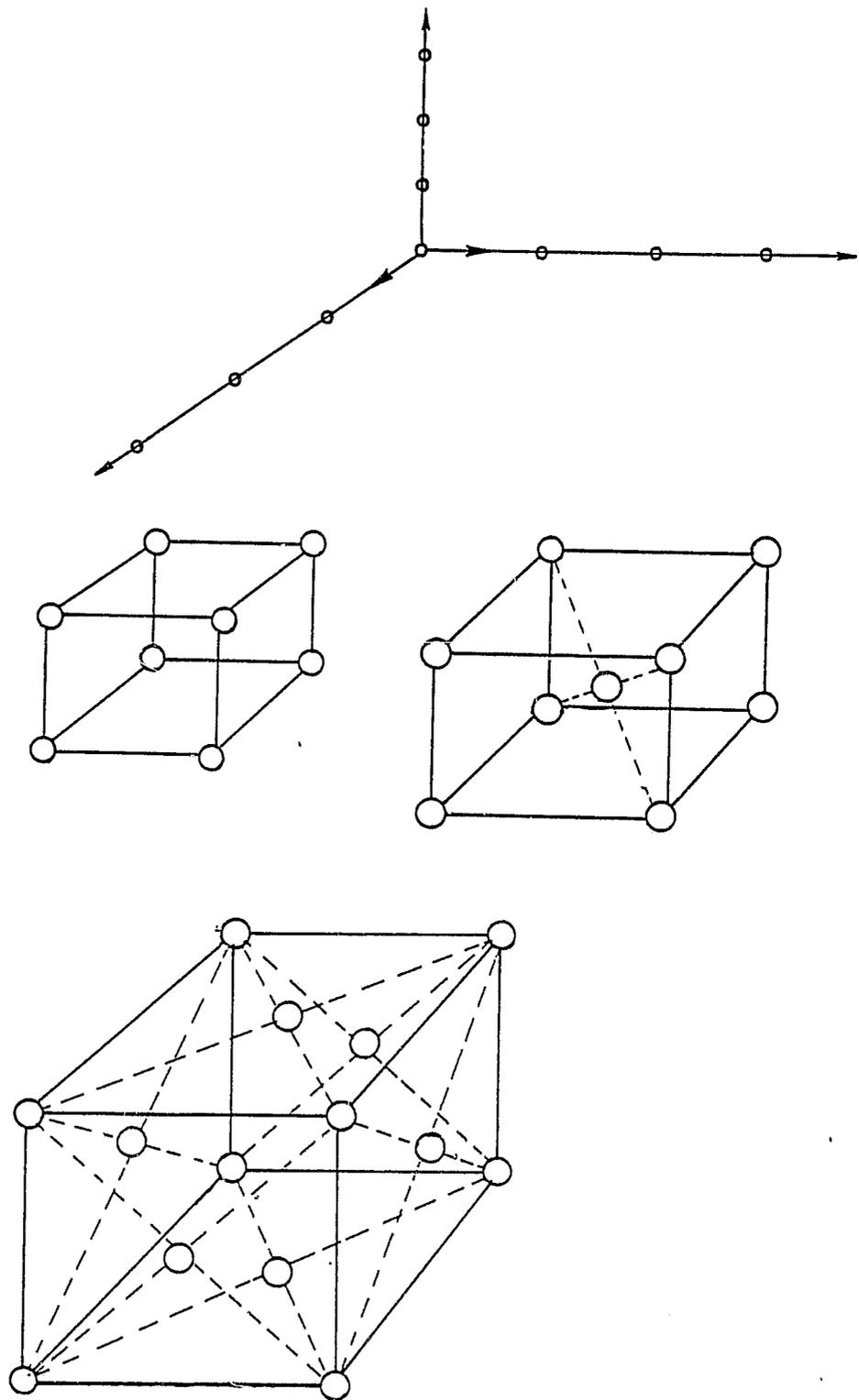
Figure 21. Basis vectors for P,I,F lattice structures.
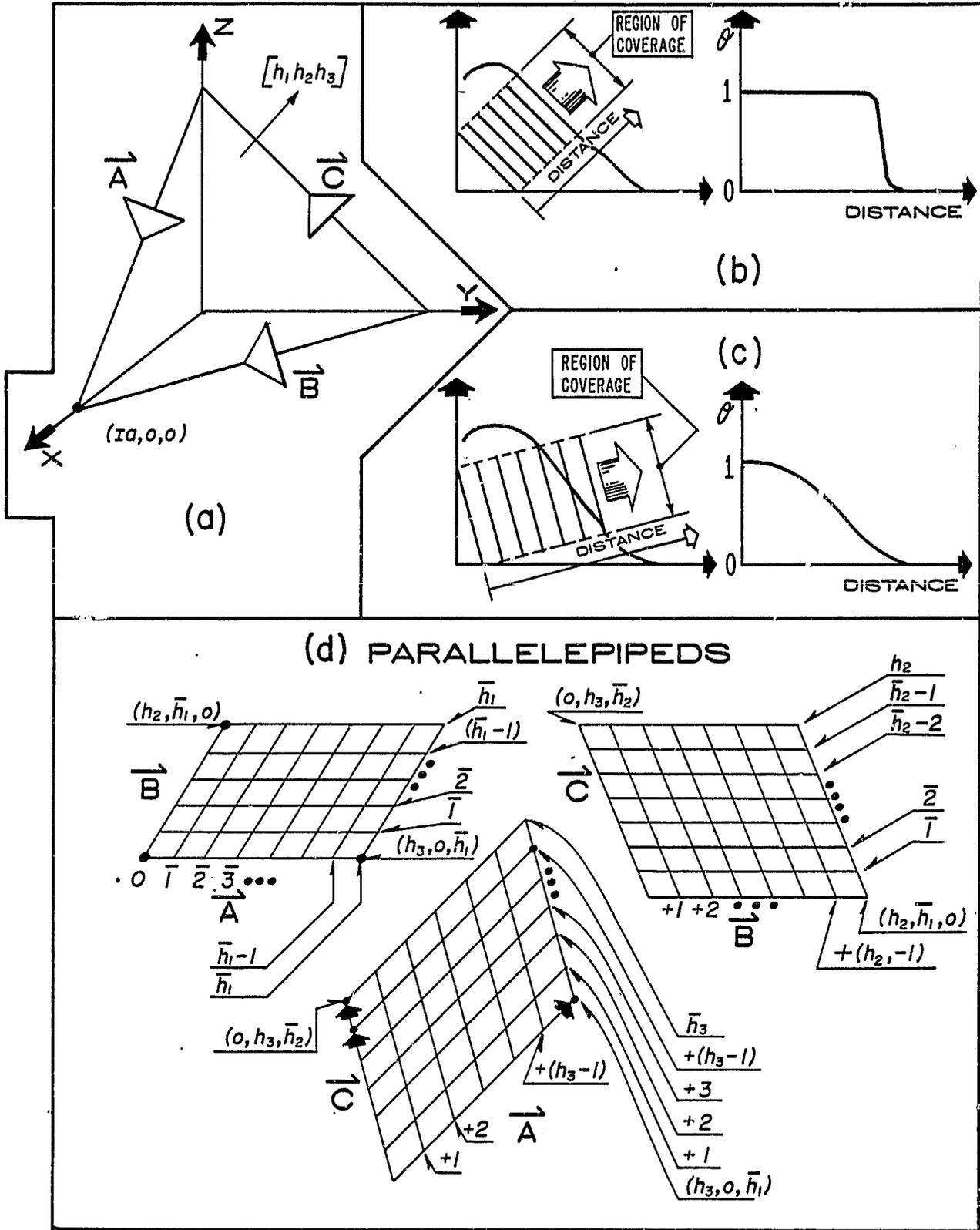
Figure 22. Crystal planes (a) their orientation and coverage with distance
(b) and (c), and (d) $\vec{A},\vec{B}$, $\vec{C},\vec{A}$ and $\vec{B},\vec{C}$ primitive cells.

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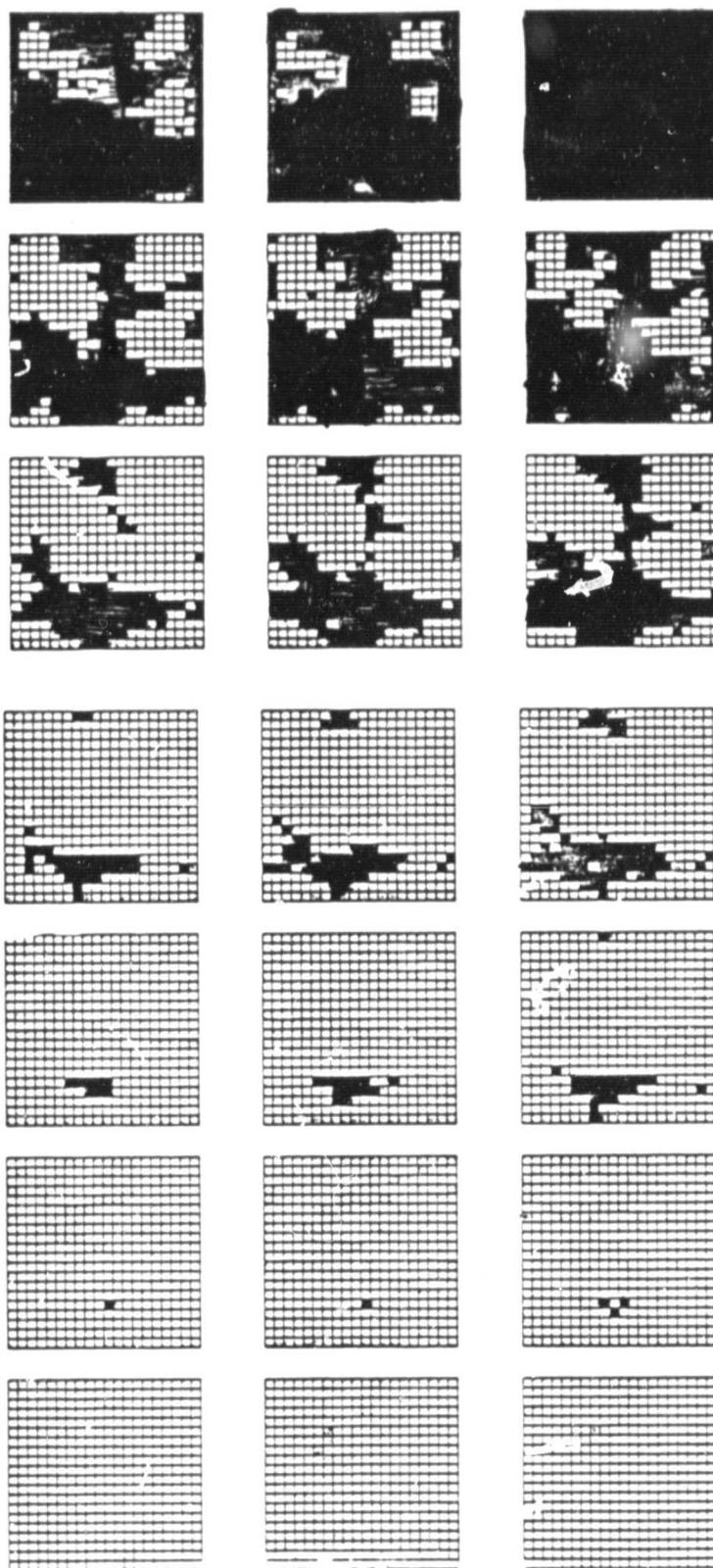
Figure 23. Graphic output from computer program. Snapshots are read from top to bottom and right to left. Each snapshot represents 0.1 sec., R_d = 0.556 nm/sec., Δt = 10^{-4} sec. (1,000 samples of each surface adatom during each snapshot interval), T = 600 K, (100) surface, U_o = -3.87 eV, ΔHads = 1.7 eV, Q_d = 0.7 eV, U_m = -1.0 eV, n = 10^8 (Boltzmann ordered statistic parameter).