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TRIDYN_FZR User Manual

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The present report contains the User Manual of the FZR version of the dynamic binary-collision computer simulation code TRIDYN. The present version of the code is based on TRIDYN Vs. 4.0 by W.Möller and W.Eckstein, Department of Surface Physics, Max-Planck Institute of Plasma Physics, Boltzmannstraße 2, 85748 Garching, Germany (1989). Modifications, in particular for PC implementation, quasi-dynamic display and the input dialog have been performed at the Institute of Ion Beam Physics and Materials Research by V.Kharlamov, T.Schwieger, M.Posselt, and W.Möller (1995-2001).

General remarks

TRIDYN simulates the dynamic change of thickness and/or composition of multicomponent targets during high-dose ion implantation or ion-beam-assisted deposition. It is based on TRIM, using the binary collision approximation (BCA) model for ballistic transport.

The main fields of application of TRIDYN include high fluence ion implantation, ion beam synthesis, sputtering and ion mixing of polyatomic solids, ion-beam or plasma assisted deposition of thin films, and ion-beam or plasma assisted etching.

Ballistic effects such as projectile deposition and reflection, sputtering, and ion mixing are computed for a target at zero-temperature. Radiation damage is not taken into account. The target and the grown layers are assumed to be amorphous. Each simulated projectile ("pseudoprojectile") represents a physical increment of incident fluence (incident particles per unit area). Up to 5 different atomic species in the target and/or in the beam may be considered, with different energies and angles of incidence for the beam components. Initially homogeneous as well as initially inhomogeneous and layered targets may be treated.

TRIDYN allows to calculate the depth profiles of all atomic species in the target as function of the incident fluence. Additionally, sputtering yields, total areal densities, surface concentrations and re-emitted amounts are calculated as function of fluence, as well as the surface erosion (when sputtering prevails) or the grown layer thickness (in the deposition regime)

The physical background of TRIDYN is described in the papers given in the refs. 1-4. A simple diffusion procedure, which is described in this manual, can be included in addition to ballistic transport of atoms.

TRIDYN covers only non-thermal processes. Due to the binary collision approximation, its lower energy limit is in the order of 10 eV. Nevertheless, experience shows that also collisional processes with slightly lower characteristic energies, such as sputtering, are predicted quite accurately. The upper energy limit is given by feasible times of computation. Nevertheless, TRIDYN is less suitable for energies in the MeV range and above. (It does not contain a collision frequency reduction such as in TRIM for higher energies.)

The following files are available to run TRIDYN_FZR:

input.f and input.exe – source code and dialog program for preparing the input files
elements.dat – file containing atomic data of the elements
tridynfzr.f and tridynfzr.exe – source code and executable program

Running the Programme (under MS-DOS Window)

Step 1: Creating Standard Input Files

Dialog using the program **input.exe,** Command: *input.exe*
Creates namexxxx.IN and optionally namexxxx.LAY.

Note! For all questions "(Yes/No?)", the "Yes" answer can be chosen by small or capital "Y" or by pressing the "Enter" button, and the answer "No" can be chosen by small or capital "N".

Input of parameters for beam and target components

At first, the name of the run to be performed (4 ASCII characters, example: AlN5) is prompted. The file "namexxxx.IN" will contain all necessary input information excluding the target structure information in the case of an inhomogeneous target. Then, prompts for the beam components, their energies and angles of incidence, fractions in the beam, maximum possible fractions in the target, energy parameters (bulk binding energies, surface binding energies), and atomic volumes appear. During the input of energy and atomic volume parameters, the values for pure elements from the file "elements.dat" are proposed. If the maximum target fraction of any component is set to less then 100 %, a "diffusion" model can be chosen, with "Yes" for diffusion of excess atoms to the nearest depth interval with an atomic fraction less than the maximum one, and "No" for reemission of excess atoms. Subsequently, target components and their parameters are prompted.

Input of calculation and target parameters

The total fluence and the corresponding number of pseudoprojectiles are prompted, followed by the target thickness, the thickness for dynamic simulation (in which the dynamic change of target composition is considered), and the number of depth intervals within the range for dynamic simulation. Subsequently, the beam and target properties are prompted. Three different types of inputs for the initial target structure are possible:

Homogeneous target: The initial target is considered as homogeneous.

Inhomogeneous target from a file: This option allows the use of a target structure obtained from a previous calculation. The name of the output file namePRxx.DAT of the previous calculation, which contains the depth profiles of the atomic components, is prompted. This file must be in the current directory. From this, the input file "namexxxx.LAY" is created. **Be careful with this option!** The number of ion beam and target components and their sequence must be the same as in the previous calculation. If necessary a beam component can be "switched off" by

setting its fraction in the beam to zero. Check that the depth for dynamic simulation, the number and width of depth intervals and other parameters are the same as in the previous simulation.

Layered Structure: An additional dialogue is set up to construct a layered structure on top of the substrate, using the target elements which have been defined in the first part of the input dialogue.

General Note! Not all parameters of the simulation are prompted during the input dialog. Some of the default parameters of the standard input file "namexxxx.IN" are not optimized for an efficient simulation. See notes below for an appropriate choice of all input parameters, which can be adjusted by editing the standard input file. For example, the standard choice of the cutoff energies is always on the safe side, but will generally cause unnecessarily long computing times. Moreover, it is often inconvenient to use the input dialog program repeatedly, such as in the case of performing a series of calculations with similar parameters. Therefore, the input file "namexxxx.IN" should preferably be edited directly, once it is available.

Step 2: Running the Simulation

The following input files are necessary for starting the simulation (see above):
a) in the case of a homogeneous target : "namexxxx.IN" (e.g. AlN5xxxx.IN)
b) in the case of an inhomogeneous target or a layered structure: "namexxxx.IN" (e.g. AlN5xxxx.IN) and "namexxxx.LAY" (e.g. AlN5xxxx.LAY)
Run of the simulation code **tridynfzr.exe:** Command: *tridynfzr.exe < namexxxx.IN*
(Example: tridynfzr.exe < AlN5xxxx.IN)
During the run, information about the status of the calculation appears on the screen.

Input Data

The input file **"namexxxx.IN"** contains the following variables:

Line 1: namexxxx.IN
Line 2: PPLOT
Line 3: IFOUT
Line 4: NH, IDOUT, IQOUT, NCP, IDREL, IQ0, IRC0, IRAND, JCP1, JCP2, JFRP, JNRM
Line 5: FLC, INEL, IWC, IDIFF
Line 6: TT, TTDYN, NQX, DSF, IQXN, IQXX, IMCP
Line 7: ZZ(1), M(1), BE(1), ED(1), EF(1), QU(1), DNS0(1), CK(1)
Line 8: E0(1), ALPHA0(1), QUBEAM(1), QUMAX(1), SBV(1,1),...,SBV(1,NCP)
Line 9: ZZ(2), M(2), BE(2), ED(2), EF(2), QU(2), DNS0(2), CK(2)
Line 10: E0(2), ALPHA0(2), QUBEAM(2), QUMAX(2), SBV(2,1),...,SBV(2,NCP)
Line 11: ...

The names used above are the same as in the TRIDYN_FZR source code.

Name of variable	Description	Parameter range or meaning Default settings
namexxxx.IN	the name of input file. The first part ("name") is used for the creation of all output files	Part "name" consist of 4 ASCII characters
PPLOT	Decides whether plots with intermediate results of the simulation appear in a separate window after each 20% progress of the calculation	Plots appear: y Plots do not appear: n
IFOUT	the number of pseudoprojectile histories after which the status messages appear on the screen	Integer, $0 < IFOUT < NH$; Default: $IFOUT = NH/20$
NH	total number of pseudoprojectiles	Integer; $NH > 0$
IDOUT	the number of pseudoprojectile histories after which integral data (files nameSRFC.DAT, ... – see below) are written	Integer; $0 < IDOUT < NH$; Default: $IDOUT = NH/5$
IQOUT	the number of pseudoprojectile histories after which the profile output files namePRxx.DAT are created	Integer; $NH/70 < IQOUT < NH$; Default: $IQOUT = NH/5$
NCP	total number of components	Integer; $2 \leq NCP \leq 5$
IDREL	index of suppression of dynamic relaxation	Integer; Default: 0 (>0 – suppression of dynamic relaxation; <0 - suppression of dynamic relaxation and cascades)
IQ0	index of structure type	Integer: 0, -1 (0 – homogeneous target; -1 – inhomogeneous target)
IRC0	index for treatment of recoil atoms in cascade	Integer; Default: -1 (<0 – "subthreshold recoils free"; ≥ 0 – "subthreshold recoils bound"
IRAND	initial random number for the random number generator	Integer; $IRAND > 0$; Default: 147483647
JCP1, JCP2	suppression of recoils of components with number between JCP1 and JCP2	Integer; $0 \leq JCP1 < JCP2$, $1 \leq JCP2 \leq 4$; Default: JCP1=0, JCP2=1 (if JCP1=0 – recoils of all components are treated)
JFRP	generation of Frenkel pairs for components with number $\geq$ JFRP (only meaningful for "static" output – see below)	Integer; $1 \leq JFRP \leq 5$; Default: 1

JNRM	output of profiles for components with number ≥ JNRM (only meaningful for "static" output – see below)	Integer; 1≤JNRM≤5; Default: 1
FLC	total fluence of all projectiles (10^{16}/cm^2)	Real; FLC>0
INEL	index for model of inelastic interaction	Integer: 1, 2, 3; Default: 1 (1 – inelastic interaction nonlocal; 2 – local; 3 – equipartition)
IWC	maximum order of weak projectile-target collisions	Integer: 1, 2, 3 ; Default: 1
IDIFF	index of "diffusion" model for atoms exceeding maximum atomic fraction (see QUMAX below)	Integer: 0, 1; (0 – diffusion and reemission; 1 – reemission)
TT	target thickness (Å)	Real; TT>0
TTDYN	depth range for dynamic simulation (Å)	Real; TTDYN>0
NQX	number of depth intervals within depth for dynamic simulation	Integer; 100≤NQX≤500
DSF	averaging depth for surface composition (Å)	Real; 0≤DSF≤TTDYN
IQXN, IQXX	profile output only for depth intervals with numbers between IQXN and IQXX	Integer; 0≤IQXN≤IQXX; 1≤IQXX≤NQX Default: IQXN=0, IQXX=NQX (if IQXN=0 – output for all intervals)
IMCP	Number of component for calculation of the moments of the depth distribution (no output in present version)	Integer; 0≤IMCP≤5; Default: 0 (if IMCP=0 – no moment calculation)
ZZ(I)	atomic number of component number I	Integer value in real format; 1≤ZZ(I) ≤92
M(I)	mass (in a.m.u.) of component number I	Real; M(I)>0
BE(I)	bulk binding energy of component number I (eV)	Real; BE(I)>0
ED(I)	relocation threshold energy of component number I (eV)	Real; ED(I)>0
EF(I)	cut off energy (eV) (atom with energy falling below this value is considered to be stopped);	Real; EF(I)>0; Default: 0.1
QU(I)	fraction of component number I in the target (substrate);	Real; 0≤QU(I) ≤1; (For beam component default: 0)

DNS0(I)	atomic density of component number I (10^{24}/cm^3) (DNS0=1/V$_I$, where V$_I$ is the volume occupied by atom of component number I)	Real; DNS0(I)>0
CK(I)	electronic stopping correction factor	Real; CK(I)>0; Default: 1
E0(I)	incident energy of component number I (eV)	Real; E0(I)≥0
ALPHA(I)	angle of incidence of component number I with respect to the surface normal	Real; 0≤ALPHA(I) ≤90
QUBEAM(I)	fraction of component number I in the beam	Real; 0≤QUBEAM≤1 (For target component QUBEAM(I)=0)
QUMAX(I)	maximum fraction of component number I in the target	Real; 0≤QUMAX(I) ≤QU(I)
SBV(I,J)	surface binding energy matrix for component number I with respect to surface component number J (J=1, NCP) (eV)	Real; Default: SBV(I,J) are equal for all components J

The default values are recommended to be used for all variables which are not prompted during the input dialog.

Choice of Input Parameters – Hints and Formulas

1. Target Intervals and Thickness

The thickness of the initially equidistant depth intervals, which is equal to TTDYN/NQX, should be small enough to allow for a sufficient resolution within the depth range of interest. However, too thin intervals might result in an artificial broadening due to the algorithm of interval splitting and combination. A choice below about 2 Å is not meaningful in view of the typical atomic distances. The stability of the results against the interval thickness should always be checked.

The range of dynamic relaxation, TTDYN, may be larger than the target thickness, TT. This is helpful, if the modification (e.g. ion mixing) of a thin layer by a high-energy ion beam, with a range much larger than the depth range of interest, shall be simulated. In this way, the high-energy pseudoprojectile is suppressed after the passage through TT, saving computer time, and the depth range of interest can be resolved sufficiently.

2. Total Fluence and Number of Pseudoprojectiles

Mostly, one will aim at reducing computer time by reducing the number of pseudoprojectile histories at a given total fluence. However, the statistical quality and the precision of the results is deteriorated simultaneously. A fluence increment of 10^{12} cm^{-2} per pseudoprojectile (e.g., 10000 pseudoprojectiles at a total fluence of 10^{16} cm^{-2}) is normally a reasonable initial choice. The statistical quality can be checked after the termination of the run by means of the output quantity MAXCHA (see below). The stability of the results against a variation of NQX should be checked.

3. Energy Parameters

TRIM, and correspondingly TRIDYN, are BCA simulations with only a repulsive interaction potential. Therefore, in contrast to classical dynamics simulations, "solid state" energy parameters have to be defined additionally.

As a general remark, the energy parameters should not be misused as fitting parameters, e.g. in order to reproduce experimental values. They should rather be chosen according to the best knowledge and according to TRIM and TRIDYN conventions as described in the following.

3.1 Cutoff Energy

The cutoff energies, EF(I), determine the energy at which any pseudoparticle (projectile or atom in a collision cascade) is stopped. Obviously, very long computation times result from very low cutoff energies, so that these should be chosen as high as possible. The upper limits depend on the problem itself. For example, if a high-energy deposition profile (as, e.g., for MeV ion beam synthesis where sputtering is negligible) shall be simulated, a very high cutoff energy (sometimes up to several keV) can be chosen, being only limited by the artificial distortion of the resulting profile at a too high cutoff energy. In general, the choice of the cutoff

energies must be consistent with the characteristic energies of the governing processes. For example, if sputtering is to be treated correctly, the cutoff energies of the target components must be equal or less than the surface binding energies SBE(I) (see below), so that the surface binding energies are a good choice also for the cutoff energies. In order to further reduce the computer time for certain problems, it may be adequate to increase the cutoff energy of a projectile according to the energy transfer to the target atoms, resulting in

$$EF_{proj} = \frac{(m_{proj} + m_{t\,arg\,et})^2}{4m_{proj}m_{t\,arg\,et}} SBE_{t\,arg\,et}^{min}$$ (1)

as, e.g., for gaseous projectiles which are not trapped in the target (see 4.)

Note! In general, it is not justified to identify the cutoff energies with the displacement threshold energies (see 3.4) which are in the order of several 10 eV. This would reduce the computing time significantly, but suppress all cascade development below these energies, and thus, e.g., result in a drastic underestimation of sputtering.

3.2 Bulk Binding Energy

In a BCA simulation, the bulk binding energy, BE(I), is subtracted from the energy transfer to the recoil atom before it is set in motion. A well-defined value for this energy is difficult to obtain. Therefore, it is often simply set to zero, with good results, e.g., for sputtering yields if other standard parameters as described here are chosen. It is also known from TRIM experience that an increase of the bulk binding energies to up to a few eV requires a corresponding decrease of the surface binding energies in order to obtain the same sputtering yields. It is recommended to set the bulk binding energies to the default value of zero.

3.3 Surface Binding Energy

The surface binding energies determine critically the sputtering yields. Theoretically, the sputtering yield is proportional to the inverse of the surface binding energy. In TRIDYN, the effective surface binding energy of each target component can be chosen in dependence on the actual surface composition. With c_j denoting the surface atomic fractions of the target atoms j $(1 \leq j \leq NCP,\ \Sigma c_j = 1)$, the surface binding energy of a surface atom i is given by

$$SBE_i = \sum_{j=1}^{NCP} SBV_{ij} \cdot c_j$$ (2)

with the matrix components SBV_{ij}. Eq. (2) includes the simple choice of surface binding energies which are independent of the surface composition, by the default setting $SBV_{ij} = SBE_i$ for all components j.

In the following, recipes of increasing complexity will be given for the choice of the surface binding energies.

3.3.1 Neglecting the projectile species at the surface

For some applications, the surface composition of a target does not change significantly during the simulation, as, e.g., for high-energy or low-fluence implantations, or inert gas bombardment where the gas concentration is neglected (see 4.) In such cases, the choice of the surface binding energy of the projectile species is not critical. A reasonable choice is

$$SBE_{proj} = EF_{proj} \qquad (3)$$

3.3.2 Enthalpy of Sublimation

For the prediction of the sputtering yield of monoatomic substances by TRIM, the choice of the sublimation enthalpies ΔH^s for the surface binding energies has proven to be successful. For each element the sublimation enthalpy given in the file **elements.da**t is taken as the default value. For multicomponent solids one might also choose as the most simple approximation

$$SBE_i = \Delta H_i^s \qquad (4)$$

This simple model is also a good approximation for multiatomic targets with low heats of fusion, such as metallic alloys.

$$SBV_{ij} = \Delta H_i^s \qquad \textit{for all j} \qquad (5)$$

3.3.3 Nonreactive Gaseous Components

It is often difficult to define the surface binding energy of a nonreactive gaseous component, due to the very low and often unknown enthalpy of physisorption. Ideally, on would tend to set

$$\Delta H_{gas}^s \rightarrow \ \textbf{0} \qquad (6)$$

However, this choice would require consistently low cutoff energies (see 3.1) and result in long computing times. A general recipe cannot be given. The stability of the results against the choice of the surface binding energy should be checked.

3.3.4 Solid-Solid Compounds (Constant Surface Binding Energy)

The following recipes shall be restricted to two-component targets A_nB_m. With respect to eq. (4), a more realistic approach is to take into account the heat of formation of a specific compound, but still to define surface binding energies being associated to the individual atoms, independent of the actual surface composition. Conservation of energy requires

$$n \cdot SBE_A + m \cdot SBE_B = n \cdot \Delta H_A^s + m \cdot \Delta H_B^s + \Delta H^f \qquad (7)$$

where ΔH^f denotes the formation enthalpy per molecule of the compound. If the heat of formation is small, it might simply be added to the enthalpy of sublimation of one of the constituents, e.g., B. This results in

$$SBE_A = SBV_{AA} = SBV_{AB} = \Delta H_A^s$$

$$SBE_B = SBV_{BA} = SBV_{BB} = \Delta H_B^s + \frac{1}{m}\Delta H^f$$

$$(8)$$

This formalism may also be employed if ΔH^f is large, but if the surface composition remains far from the pure component B. Then, with eq. (8), the surface binding energy of the pure A surface is approximately correct, and eq. (7) is fulfilled. Physically, this model is justified, if, e.g., preferential sputtering or thin film deposition result in a surface composition between that of the stoichiometric compound and an enrichment of the component A.

Example: Preferential sputtering of TaC by He at keV energies results in an enrichment of Ta at the surface. Therefore, the choice of the surface binding energies should be good for the compound itself and for the limit of a pure Ta surface. With $\Delta H^s_{Ta} = 8.1\ eV$, $\Delta H^s_C = 7.41\ eV$, and $\Delta H^f_{TaC} = 1.54\ eV$, it is reasonable to set $SBE_{Ta} = SBV_{TaTa} = SBV_{TaC} = SBV_{TaHe} = 8.1\ eV$, and $SBE_C = SBV_{CTa} = SBV_{CC} = SBV_{CHe} = 8.95\ eV$, and for the projectile component $SBE_{He} = SBV_{HeTa} = SBV_{HeC} = SBV_{HeHe} = EF_{He} = 9\ eV$ (see 3.3.1 and eq. (1)).

3.3.5 Solid-Gas Compounds (Constant Surface Binding Energy)

If one of the constituents of the target A_nB_m, e.g. B, is from a diatomic gas, its enthalpy of dissociation ΔH^{diss} has to be taken into account. Then, in analogy to eq. (7)

$$n \cdot SBE_A + m \cdot SBE_B = n \cdot \Delta H^s_A + \Delta H^f + \frac{m}{2} \Delta H^{diss} \qquad (9)$$

As the gaseous component will normally not be enriched significantly, a proper choice is

$$SBE_A = SBV_{AA} = SBV_{AB} = \Delta H^s_A$$

$$SBE_B = SBV_{BA} = SBV_{BB} = \frac{1}{m} \Delta H^f + \frac{1}{2} \Delta H^{diss} \qquad (10)$$

Example: During the ion beam synthesis of Si_3N_4 by nitrogen bombardment of silicon the surface stoichiometry remains between pure Si and the stoichiometric Si_3N_4 compound. With $\Delta H^s_{Si} = 4.7\ eV$, $\Delta H^{diss}_{N2} = 9.85\ eV$, and $\Delta H^f_{Si3N4} = 7.8\ eV$, one obtains $SBE_{Si} = SBV_{SiSi} = SBV_{SiN} = 4.7\ eV$, and $SBE_N = SBV_{NSi} = SBV_{NN} = 6.95\ eV$.

In some cases, an atomization enthalpy ΔH^a per atom of the gaseous component can be found in the literature (see, e.g. ref. 5). Then

$$SBE_B = SBV_{BA} = SBV_{BB} = \Delta H^a_B \qquad (11)$$

This is strictly valid only if the deviation of the surface composition from stoichiometry is small.

3.3.6 Solid-Solid Compounds (Variable Surface Binding Energy)

For a diatomic compound A_nB_m, eq. (2) reads

$$SBE_A = SBV_{AA} \cdot c_A + SBV_{AB} \cdot c_B$$

$$SBE_B = SBV_{AB} \cdot c_A + SBV_{BB} \cdot c_B \qquad (12)$$

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Physically, the matrix elements SBV_{ij} denote the interaction energies between atoms i and j. Therefore, $SBV_{ij} = SBV_{ji}$ has been assumed. For a solid-solid compound, they are related to the enthalpies of formation and sublimation, ΔH^f and ΔH^s, respectively. For $c_A = 1$ and $c_B = 0$ and vice versa, the pure components A or B are given, so that

$$SBV_{AA} = \Delta H_A^s$$

$$SBV_{BB} = \Delta H_B^s \tag{13}$$

The combination of eqs. (7,12,13) yields for the stoichiometric compound with $c_A = n/(n+m)$ and $c_B = m/(n+m)$

$$SBV_{AB} = SBV_{BA} = \frac{1}{2}\left(\Delta H_A^s + \Delta H_B^s\right) + \frac{n+m}{2nm}\Delta H^f \tag{14}$$

Compared to eq. (8), eqs. (13,14) are of better symmetry and thus more rigorous, but still only valid if the deviation from the stoichiometric compound is not too strong. Alternatively, by setting $c_A = 0$ and $c_B = 1$ in eq. (12 top) or vice versa in eq. (12 bottom), the non-diagonal matrix elements may be identified with the sorption energy of A on the elemental B surface, and vice versa, which are not symmetric in general. Then

$$SBV_{AB} = \Delta H_{AB}^{sorp}$$

$$SBV_{BA} = \Delta H_{BA}^{sorp} \tag{15}$$

where $\Delta H^{sorp}{}_{ij}$ denotes the sorption enthalpy of atom i on the elemental surface j. Unfortunately, the sorption enthalpies are not readily available in literature, so one will generally prefer the approach of eq. (14), except when treating specific problems of surface physics.

3.3.7 Solid-Gas Compounds (Variable Surface Binding Energy)

If in a diatomic compound A_nB_m one of the components is from a diatomic gas, e.g., B, one may neglect any interaction of B atoms in the surface. (Otherwise, they would react and form a volatile molecule.) Therefore

$$SBV_{AA} = \Delta H_A^s$$

$$SBV_{BB} = 0 \tag{16}$$

In analogy to 3.3.6, the combination of eqs. (9,12,15) yields for the stoichiometric compound

$$SBV_{AB} = SBV_{BA} = \frac{1}{2}\Delta H_A^s + \frac{n+m}{2nm}\Delta H^f + \frac{n+m}{4n}\Delta H^{diss} \tag{17}$$

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In summary, the matrix formulation for the surface binding energies (eq. (2)) allows a large variety of different models for the surface binding as discussed in 3.3.1-3.3.7. Similar formalisms can be derived for more than two components. Other models might be appropriate for specific problems.

3.4 Relocation Threshold Energy, Subthreshold Recoils

The relocation of recoils is steered by the recoil index IRC0 and the relocation threshold energies ED(I). The relocation threshold critically determines the amount of ion mixing, but also the shape of compositional profiles resulting from low-energy implantation and/or preferential sputtering. The width of collisional mixing profiles scales as $ED^{-1/2}$.

The conventional model assumes that a Frenkel pair can only be formed if the interstitial atom is relocated far enough from its original lattice site, corresponding to a minimum energy transfer when it is created. This minimum energy transfer is denoted as the displacement threshold energy, which is in the order of several 10 eV. This model can be implemented by identifying the relocation threshold energies with the displacement threshold energies, and setting subthreshold recoils "bound" with IRC0>0. (In the simulation, this causes all recoil atoms to be followed down to their cutoff energy, but to be restored at their original sites after cutoff, provided their initial energy had been below the relocation threshold energy. In this way, in the subthreshold regime only mass transport is suppressed, whereas cascade evolution and momentum transport are maintained. Thus, e.g., sputtering is not influenced by the choice of the relocation threshold.)

It should be noted that the concept of a displacement threshold is strictly valid only for a perfect and nondamaged crystal. In an amorphous substance or in a solid being subjected to high-fluence ion bombardment (which is the standard application of a TRIDYN simulation), relocation thresholds might be significantly lower. Well-based data cannot be given. However, according to experience with, ion mixing and preferential sputtering simulations and their comparison to experimental findings, a relocation threshold energy of 8 eV has turned out to be successful in a number of different systems, such as metallic compounds at low temperature and oxides, so that this value is recommended.

For each element the relocation threshold energy given in the file **elements.dat** is taken as the default value.

The "free" subthreshold recoil option (IRC0<0) gives additional flexibility. In this case, all recoils remain at the position where the cutoff energy is reached. Thus, the cutoff energies (see 3.1) serve as effective relocation thresholds. Then, the displacement threshold energies can be chosen independently, with corresponding results in the "static" output file (see below).

Note! With the "free" subthreshold recoil option (IRC0<0), make sure that sputtering is not influenced by the choice of excessively high cutoff energies.

4. Maximum Concentration, Reemission, Simplified "Diffusion" Model

For each component, a maximum atomic fraction in the target can be defined by QUMAX(I). This is of particular interest if gaseous species are involved.

4.1 Nonreactive Gas Implantation

An implantation of nonreactive gaseous atoms is often limited by a saturation in the implanted region, which often depends on the implantation temperature. Physically, sizeable amounts of gas reside in gas-filled voids. If the saturation concentration is known from experiment, it can be inserted into the TRIDYN simulation. If it is not known, it is preferred to fully ignore the implanted species (such as for ion mixing, preferential sputtering and nonreactive ion-assisted deposition) using QUMAX = 0. The opposite case of an unlimited implantation (QUMAX = 1) is problematic for several reasons: In addition to an unrealistically high gas incorporation, a large fraction of the collisional energy will be transferred to the gaseous component, thus reducing, e.g., the sputtering yields of the other components.

4.2 Solid-Gas Compound

In a solid-gas compound, the atomic fraction of the gaseous component is often limited to a value close to the stoichiometric fraction. Excess gas atoms behave similarly to nonreactive gases (see 4.1). Therefore, if not known better, the maximum atomic fraction should be chosen equal to the stoichiometric value.

Example: For the implantation of nitrogen into silicon with the stoichiometric compound Si_3N_4, $QUMAX_{Si} = 1$, $QUMAX_N = 0.571$.

If an additional gas take-up, such as in gas-filled voids, is known from experiment, QUMAX may be increased correspondingly.

4.3 Excess Atoms

Using the parameter IDIFF, there are two possibilities to steer the behavior of atoms whose concentration exceeds the maximum atomic fraction QUMAX. The simplest choice is to discard them (IDIFF = 1), which corresponds physically to a direct reemission into the vacuum. Alternatively, a simple "diffusion" model can be employed (IDIFF = 0). In this case, excess atoms are moved from their original depth interval to the nearest interval with a concentration of this species below QUMAX, within the dynamic range TTDYN. If the concentration is QUMAX in all depth intervals, the excess atoms are reemitted.

Note! The simple diffusion picture is realistic only for some specific systems, such as the formation of a buried oxide in silicon by oxygen implantation. It is not appropriate for a corresponding formation of a buried nitride. This indicates that any generalization of the simple diffusion model is not justified.

5. Atomic Density, Depth Scale

For monoatomic materials the atomic densities of the pure element can be used. The corresponding atomic volumes are taken from the file **elements.dat**. In the case of compound materials, TRIDYN calculates the local total atomic density *DNS* linearly from the atomic densities of the individual components *DNS0* according to

$$\frac{1}{DNS} = \sum_{j=1}^{NCP} \frac{c_j}{DNS0_j} \tag{18}$$

Similar to the choice of surface binding energies (see 3.3), in dependence on the actual problem it has to be decided which limiting cases shall be reproduced correctly.

In a solid-solid compound with little chemical interaction, the choice of the pure element atomic densities for DNS0(I) trivially reproduces the atomic densities of the pure elements and yields a good approximation for the whole range of concentrations.

In a highly covalent solid-solid compound or in a solid-gas compound, normally the density of the stoichiometric compound and that of one of the constituents should be reproduced correctly. (In a solid-gas compound, the atomic density of the pure gaseous component is ill-defined, anyway.)

Again, the following recipe shall be restricted to a two-component compound A_nB_m. Starting from the mass density ρ_A of the "principal" component A (the nongaseous component or the component for which the pure elemental density shall be reproduced correctly), and the mass density of the compound ρ_{AnBm}, the corresponding atomic densities are

$$DNS0_A = \frac{\rho_A L}{M_A} \tag{19}$$

$$DNS_{AnBm} = (n+m)\frac{\rho_{AnBm} L}{nM_A + mM_B} \tag{20}$$

with L denoting Avogadro's number and M the atomic masses. Then, the atomic density of the non-principal component is calculated from eq. (18) according to

$$DNS0_B = \left(\frac{n+m}{m}\frac{1}{DNS_{AnBm}} - \frac{n}{m}\frac{1}{DNS0_A}\right)^{-1} \tag{21}$$

Due to the definition of pseudoprojectiles which represent increments of fluence, i.e. atoms per unit area, the natural depth scale of TRIDYN is an areal density, with each depth interval given by the total number of atoms per unit area in this interval. For the resulting depth profiles, geometrical depths are calculated by dividing the areal density of each depth interval by its total atomic density according to eq. (18).

Example: The ion-beam assisted deposition of Ta_2O_5 by tantalum evaporation and oxygen ion bombardment shall be simulated. Obviously, the principal component is tantalum with $\rho_{Ta} = 16.6\ g/cm^3$ and $M_{Ta} = 180.95\ g/mole$, and according to eq. (19), $DNS0_{Ta} = 5.53 \cdot 10^{22}\ cm^{-3}$. Similarly, for the compound, $\rho_{Ta2O5} = 7.5\ g/cm^3$ and $M_O = 16.0\ g/mole$, and according to eq. (20), $DNS0_{Ta2O5} = 7.16 \cdot 10^{22}\ cm^{-3}$. From this and eq. (21), the input atomic density for the oxygen component results as $DNS0_O = 8.11 \cdot 10^{22}\ cm^{-3}$.

For the bombardment with inert gas atoms, their incorporation might cause a swelling of the material, due to high-pressure gas-filled voids. The density of the gas within these bubbles and their volume fraction are mostly unknown. Therefore, one might simply discard the swelling by

setting

$$DNS0_{InertGas} \rightarrow \quad \infty \tag{22}$$

i.e., numerically $DNS0_{InertGas} > 10^{28} \, cm^{-3}$. In this way, the presence of the gaseous component is neglected for the depth scale calculation, but not for the development of the collision cascades (unless $QUMAX = 0$ for the inert gas – see 4.)

Example: A *TaC* surface is bombarded with *He*. Due to the more efficient momentum transfer, carbon will be sputtered preferentially, so that tantalum is chosen as the principal component. Any swelling by incorporated helium shall be neglected. With $\rho_{Ta} = 16.6 \, g/cm^3$ and $M_{Ta} = 180.95 \, g/mole$, $DNS0_{Ta} = 5.53 \cdot 10^{22} \, cm^{-3}$ according to eq. (19). Similarly, for the compound, with $\rho_{TaC} = 13.9 \, g/cm^3$ and $M_C = 12.0 \, g/mole$, and, $DNS0_{TaC} = 8.68 \cdot 10^{22} \, cm^{-3}$ according to eq. (20). From eq. (21), $DNS0_C = 2.02 \cdot 10^{23} \, cm^{-3}$ and, according to eq. (22), $DNS0_{He} = 10^{30} \, cm^{-3}$.

Note! For compounds with a very high atomic density, the atomic density of the non-principal component may become negative according to eq. (21). This represents no problem for the processing in TRIDYN.

6. Incident Energies

6.1 Molecular Bombardment

In many cases, such as for molecular ion implantation or in the case of plasma-enhanced chemical vapour deposition, the incident species are molecules, e.g., A_nB_m. For each of the constituents, the beam fractions QUBEAM(I) and the incident energies E0(I) have to be defined consistently. For incident energies being sufficiently large compared the molecular binding energies, surface collisions will cause an immediate dissociation of the incident molecule. Then, the incident energy $E0_{AnBm}$ of the molecule is distributed according to the atomic masses M_A and M_B, resulting in

$$E0_A = \frac{M_A}{nM_A + mM_B} \cdot E0_{AnBm}$$

$$\tag{23}$$

$$E0_B = \frac{M_B}{nM_A + mM_B} \cdot E0_{AnBm}$$

Example: For the plasma etching of silicon, CF_3^+ ions may represent a major species. For a substrate bias of *500 V* corresponding to an incident ion energy of $E0_{CF3} = 500 \, eV$, eq. (23) yields with $M_C = 12 \, g/mole$ and $M_F = 19 \, g/mole$ $E0_C = 87 \, eV$ and $E0_F = 138 \, eV$.

6.2 Thermal Neutrals and Low-Energy Ions

Often, the incident flux consists of ions and neutral particles at thermal energies, such as in ion-assisted deposition or plasma-enhanced chemical vapor deposition. Such species can be treated in TRIDYN by setting

$$E0_{neutr} = \quad 0 \tag{24}$$

As stated above, the treatment of the collisional processes in TRIDYN is problematic for very low ion energies (about 30 eV and below). Nevertheless, the low-energy incident particles will be correctly deposited at the surface.

The user should be aware of the fact that each incident pseudoparticle is accelerated by the surface binding energy SBE(I) before entering the solid.

Output

TRIDYN provides the following output files:

#	Description	Name	Example
1	Depth profiles of the components for given values of the incident fluence. Default: xx = 00,01, 02,03,04,05, i.e.an output file is created at the beginning of the simulation and after each fluence increment of 20 % of the total fluence	namePRxx.DAT	AlN5PR04.DAT
2	Surface composition (within the averaging depth DSF) as function of incident fluence (Default cf. 1))	nameSRFC.DAT	AlN5SRFC.DAT
3	Integrated areal densities of the components (within TTDYN) as function of the incident fluence (Default cf. 1))	nameARDN.DAT	AlN5ARDN.DAT
4	Sputtering yields of the components as function of the incident fluence (Default cf. 1))	nameSPYL.DAT	AlN5SPYL.DAT
5	Accumulated reemitted fluence as function of the incident fluence (Default cf. 1))	nameREEM.DAT	AlN5REEM.DAT
6	Surface recession as function of incident fluence. A negative surface recession corresponds to a thin film deposition (Default cf. 1))	nameSRRS.DAT	AlN5SRRS.DAT
7	Output listing (input data, statistics, particle balances, "static" projectile (component 1 only) and energy deposition profiles (see remark given below)	nameOUT.DAT	AlN5OUT6.DAT

In the output listing (# 7), the lines given below the lines denoted by "areal densities and fluences" should in general be ignored for a dynamic TRIDYN run. They contain information on depth and energy deposition profiles as well radiation damage in a simple Kinchin-Pease model, integrated over the whole run. However, in static mode (IDREL<0), the simulation corresponds to a standard TRIM simulation with this output.

Test of the statistical quality and precision of the results using the parameter MAXCHA

The output listing (file nameOUT.DAT) contains the parameter MAXCHA. **For results with sufficient statistical quality and precision MAXCHA should be less than 0.05!** An increase of the number of pseudoparticles NH and a reduction of the total fluence FLC result in a decrease of MAXCHA.

Error messages

During the simulation the error messages are written on the screen and into the output listing (file nameOUT.DAT) if certain program parameters were not chosen properly. Some of the errors can stop the program before the regular end of simulation. The following error messages may occur:

1) "Projectile (recoils) range exceeds dynamic composition range. Increase TTDYN"

This message appears when the projectile or a recoil went out of the limit of dynamic composition range. The simulation is stopped after the accumulation of a definite number (default: 5 % of the number of projectiles) of such events. The depth of dynamic simulation should be increased to avoid this problem.

2) "Depth interval completely depleted. Decrease FLC or increase NH"

This message appears if the change of the composition induced by a projectile in a certain depth interval is so high, that the interval is completely depleted. The simulation is stopped after accumulation of a definite number (default: 1 % of the number of projectiles) of such events. The problem can be avoided by decreasing of total fluence or by increasing the number of ion histories (pseudoprojectiles).

3) "Deposited depth is larger than dynamic depth range. Output profile might be in error. Increase TTDYN (and NQX)"

Decrease the total fluence or increase the depth for dynamic simulation (and number of intervals if the same depth interval is required) to avoid this problem.

4) "Recoil storage capacity exceeded"

The total number of recoils for each projectile is limited by a definite number (default: 20000). If this limit is exceeded (this occurs only for very high ion energies) the program is stopped.

References

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