

Pressure-Controlled Transport of Sputtered Atoms in Thin-Film Deposition: Mean-Free-Path and Collision-Probability Analysis

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Abstract: Sputter deposition involves the generation of energetic target atoms followed by their transport through a background gas toward a substrate. This work examines the pressure dependence of that transport within a two-stage SRIM–SIMTRA framework, in which SRIM describes the sputtering of aluminium, germanium, boron, niobium, antimony and copper targets bombarded at normal incidence by argon, xenon, helium, neon and silicon ions, and SIMTRA describes the subsequent gas-phase transport. The physical link between pressure and trajectory is expressed through the mean free path and the probability of collision during the target-to-substrate flight. These relations are extended to the ballistic survival fraction, the mean collision number, the diffusion coefficient and the ballistic and diffusive transit times, and are supported by a nomenclature table, a Knudsen-number regime classification, a two-dimensional pressure–temperature map and a schematic of the SRIM–SIMTRA workflow. The analysis covers gas temperatures of 300–450 K, the interval over which the calculations were compared with previous work. All pressure-dependent figures in this paper are calculated directly from the stated analytical relations with explicitly specified illustrative parameters; they are not experimental measurements or SRIM/SIMTRA output. For an effective collision diameter of 0.36 nm, a 0.10 m flight path and 300 K, the transport moves from the transitional into the continuum regime at about 1 Pa, and the ballistic and diffusive transit-time estimates cross at a Knudsen number of 1.5.

Keywords: thin films; sputtering; Monte Carlo; sputtering yield; particle transport; SRIM; SIMTRA; pressure; temperature

1 Introduction

Sputtering is a physical vapour deposition process in which ions generated in a plasma bombard a solid target and transfer sufficient momentum to eject atoms from its surface. The emitted particles then travel through the deposition chamber and may condense on a substrate. The final film is therefore determined both by the atom-production process at the target and by the transport process between target and substrate [1–4].

These two processes can be treated as complementary numerical stages: sputtering yields for technologically relevant materials are computed with SRIM [5], and the population of atoms arriving at the substrate under changed chamber conditions is computed with SIMTRA [6]. The same two-stage approach has been used in the author's earlier Monte Carlo studies [7–9]. The calculations considered in this work cover Al, Ge, B, Nb, Sb and Cu targets bombarded by Ar, Xe, He, Ne and

Si ions, and have been compared with analytical Monte Carlo-based descriptions over sputter temperatures of 300–450 K [8].

Pressure is especially important during the second stage. Increasing the background-gas pressure increases the gas density and therefore the probability that an emitted atom collides before reaching the substrate. Such collisions change the direction and kinetic energy of the sputtered particle. SIMTRA was developed specifically to model the transport of sputtered atoms through a given chamber geometry while accounting for collisions with the background gas and their consequences for deposition profiles and arrival energies [2, 6]. The influence of pressure, target–substrate distance and other chamber parameters on the pathways of ejected atoms to the substrate has also been examined in the author's earlier Monte Carlo work [7, 9, 10].

The objective of the present paper is to describe this pressure dependence through explicit governing

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equations, a structured parameter table and a graphical interpretation of the resulting trends. The paper concentrates on the analytical description of the transport stage; the numerical SRIM and SIMTRA outputs are not repeated here, and every pressure-dependent quantity shown is calculated from the analytical relations given in Section 2.

2 Physical and numerical methodology

2.1 Sputtering yield

The sputtering yield is defined as the average number of target atoms removed per incident ion:

$$Y = \frac{N_e}{N_i}, \quad (1)$$

where N_e is the number of ejected target atoms and N_i is the number of incident ions. In SRIM-type ion–solid calculations, the yield is controlled by the projectile energy, the projectile and target masses, the collision cascade, nuclear and electronic energy loss, and the effective surface binding energy of the target [5]. The calculations considered here use normal incidence and the six target materials and five incident species listed in Table 1.

2.2 Gas-phase transport

For a dilute background gas, a useful first-order description of the collision spacing is the mean free path

$$\lambda = \frac{k_B T}{\sqrt{2} \pi d^2 p}, \quad (2)$$

where k_B is Boltzmann's constant, T is the gas temperature, d is an effective collision diameter and p is the pressure. The probability that an atom experiences at least one collision over a flight distance L is correspondingly

$$P_{\text{coll}} = 1 - \exp\left(-\frac{L}{\lambda}\right). \quad (3)$$

Equations (2) and (3) explain the qualitative pressure dependence examined with SIMTRA: increasing p decreases λ and increases P_{coll} . A complete SIMTRA result additionally depends on the chamber geometry, the energy and angular distributions of the sputtered species, the interaction potential and the full sequence of stochastic collisions [1, 2, 6].

Table 1: Species and simulation roles considered in this work.

Category	Species	Role
Targets	Al, Ge, B, Nb, Sb, Cu	Sputtered materials
Incident ions	Ar, Xe, He, Ne, Si	Bombarding species in SRIM
Transport code	SIMTRA	Target-to-substrate Monte Carlo transport
Ion–solid code	SRIM	Sputtering/ion–matter calculation
Temperature range	300–450 K	Range of the earlier comparison [8]
Incidence	Normal	Condition for the SRIM calculations

2.3 Monte Carlo implementation

Each simulated sputtered atom can be regarded as a statistical realization of an initial position, direction and energy, followed by a sequence of free-flight and collision events. This approach is appropriate because the collision locations, scattering angles and energy transfers are all probabilistic. Monte Carlo descriptions of sputtered-particle transport account for these stochastic processes and allow the effect of chamber geometry and gas-phase collisions on the arriving population to be evaluated [2, 10–14].

2.4 Gas density, cross section and flux attenuation

The mean-free-path relation of Eq. (2) can be written explicitly in terms of the background-gas number density n and an effective hard-sphere collision cross section σ . For an ideal background gas,

$$n = \frac{p}{k_B T}, \quad \sigma = \pi d^2, \quad \lambda = \frac{1}{\sqrt{2} n \sigma}. \quad (4)$$

Equation (4) is algebraically identical to Eq. (2) once n and σ are substituted. It is included because it separates the pressure dependence, through n , from the purely geometric dependence, through σ , which becomes useful if different collision diameters are assigned to the different gas species (Ar, Xe, He, Ne) listed in Table 1.

The collision probability of Eq. (3) saturates toward unity once several collisions become likely, and by itself it does not distinguish a mildly collisional trajectory from a heavily collisional one. It is therefore useful to define the complementary ballistic survival fraction, i.e. the fraction of atoms launched along a straight path of length L that reach that distance without a collision,

$$S(L) = \exp\left(-\frac{L}{\lambda}\right), \quad (5)$$

and the associated mean number of collisions accumulated over the same flight distance,

$$\langle N \rangle = \frac{L}{\lambda}. \quad (6)$$

Equations (5) and (6) add no physics beyond the single exponential model of Eq. (3); they reorganize the same collision statistics into quantities, the survival fraction and the expected collision count, that remain informative deep into the collision-dominated regime, where P_{coll} is already indistinguishable from 100%.

2.5 Ballistic and diffusive transport regimes

The Knudsen number $Kn = \lambda/L$, discussed further in Section 3, separates two limiting transport regimes. In the free-molecular limit ($Kn \gg 1$) an ejected atom travels essentially ballistically at its post-ejection speed; in the collision-dominated limit ($Kn \ll 1$) repeated small-angle deflections randomize its direction, and transport is better described as a diffusion process. A standard kinetic-theory estimate of the mean thermal speed of a particle of mass m at temperature T is

$$\bar{v} = \sqrt{\frac{8k_B T}{\pi m}}, \quad (7)$$

which, for an illustrative atomic mass $M = 60$ u, representative of a mid-mass target between Al ($M \approx 27$ u) and Nb ($M \approx 93$ u), gives $\bar{v} \approx 325$ m/s at $T = 300$ K. The associated diffusion coefficient in the collision-dominated regime follows from elementary kinetic theory as

$$D = \frac{\lambda \bar{v}}{3}, \quad (8)$$

and the characteristic ballistic and diffusive transit times over a distance L are, respectively,

$$\tau_b = \frac{L}{\bar{v}}, \quad (9)$$

$$\tau_d = \frac{L^2}{2D}. \quad (10)$$

The ballistic time τ_b is independent of pressure because it depends only on the launch speed, whereas τ_d grows linearly with pressure because $D \propto \lambda \propto 1/p$. Equating Eqs. (9) and (10) with Eq. (8) gives $\lambda = 3L/2$, so the two estimates cross at $Kn = 1.5$ independently of the gas parameters, close to the $Kn \approx 1$ boundary shown in Fig. 5. This crossover is examined quantitatively in Section 3.4.

3 Pressure dependence of the ejected-atom path

The pressure effect can be understood through the ratio $Kn = \lambda/L$, where L is a characteristic target-to-substrate

Table 2: Nomenclature.

Symbol	Definition	Unit
Y	Sputtering yield (Eq. 1)	atoms/ion
N_e, N_i	Ejected atoms, incident ions	count
λ	Mean free path (Eq. 2)	m
k_B	Boltzmann constant	J/K
T	Gas temperature	K
d	Effective collision diameter (illustrative)	m
p	Background-gas pressure	Pa
n	Gas number density (Eq. 4)	m ⁻³
σ	Collision cross section (Eq. 4)	m ²
L	Target-to-substrate flight distance	m
P_{coll}	Probability of ≥ 1 collision over L (Eq. 3)	–
S	Ballistic survival fraction (Eq. 5)	–
$\langle N \rangle$	Mean collision number over L (Eq. 6)	–
$\bar{v}$	Mean thermal speed (Eq. 7)	m/s
m	Atomic mass of the transported species	kg
D	Diffusion coefficient (Eq. 8)	m ² /s
τ_b, τ_d	Ballistic, diffusive transit time (Eqs. 9–10)	s
Kn	Knudsen number, λ/L	–

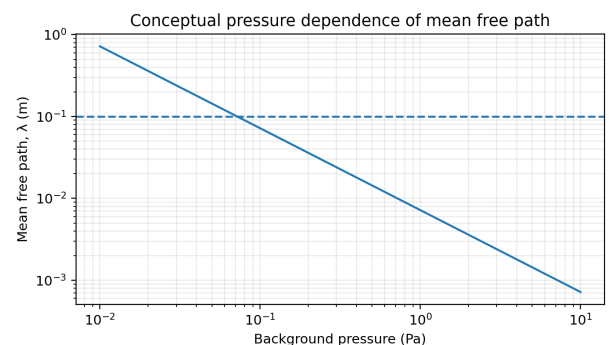


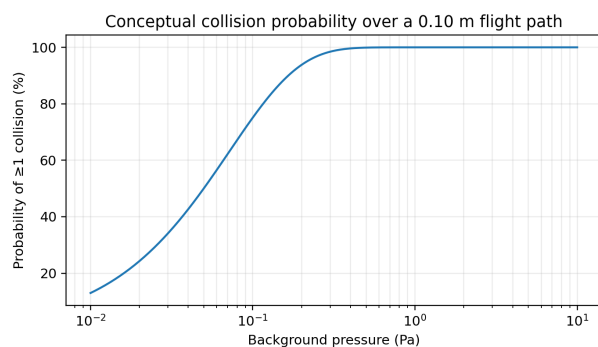
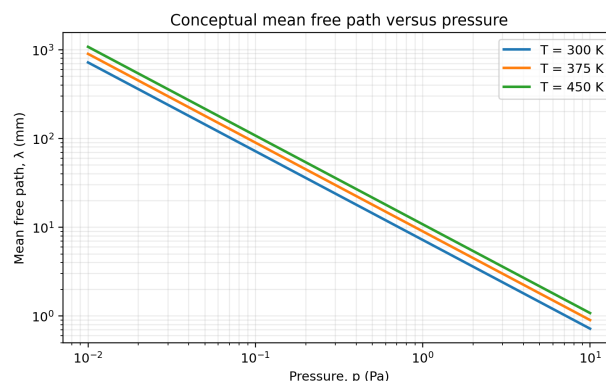
Fig. 1: Mean free path versus pressure at $T = 300$ K for an illustrative effective collision diameter $d = 0.36$ nm, calculated from Eq. (2).

distance. For $Kn \gg 1$, most atoms traverse the chamber without a collision and transport is approximately ballistic. When Kn approaches or falls below unity, collisions become increasingly important and the arriving population differs progressively from the initially emitted population [2, 6]. Figures 1–9 are calculated directly from Eqs. (2)–(10) with the illustrative parameters stated in each caption; they are analytical curves and not SRIM/SIMTRA output.

Figure 1 illustrates the inverse pressure dependence of λ . The values are calculated for an explicitly stated illustrative collision diameter; they visualize the

Table 3: Knudsen-number transport-regime classification used in this paper.

Regime	Knudsen number	Physical description
Free-molecular (ballistic)	$Kn > 1$	Most atoms cross the chamber without a collision; transport approximated by Eq. (9)
Transitional	$0.1 \leq Kn \leq 1$	Comparable collided and uncollided populations arrive; neither limiting expression is accurate
Continuum (diffusive)	$Kn < 0.1$	Atoms undergo many small-angle collisions before arrival; transport approximated by Eqs. (8) and (10)

**Fig. 2:** Probability of at least one collision over an illustrative 0.10 m flight path at 300 K, calculated from Eq. (3).**Fig. 3:** Mean free path versus pressure at three gas temperatures (300, 375 and 450 K), calculated from Eq. (2) with $d = 0.36$ nm.

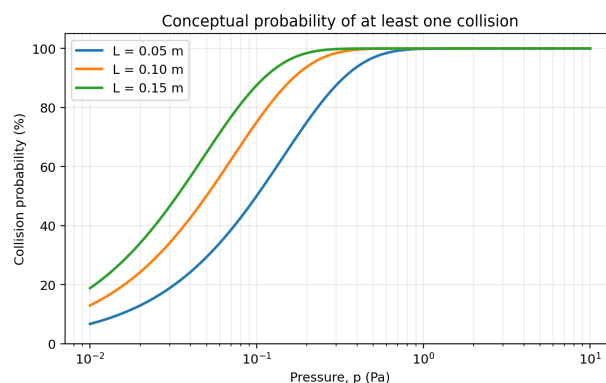
governing physics and are not intended to represent a measured property of a specific gas mixture.

Figure 2 translates the mean-free-path argument into a trajectory interpretation: as pressure rises, the chance of at least one collision along a fixed flight path increases. In a full SIMTRA calculation, multiple collisions additionally produce energy loss and angular redistribution, so the resulting deposition profile cannot be inferred from the collision probability alone.

Figure 3 extends the pressure analysis to the 300–450 K interval. At fixed pressure, increasing temperature increases the mean free path, whereas pressure remains the dominant inverse control variable. The separation among the curves follows directly from $\lambda \propto T/p$.

For a longer flight path (Fig. 4), the same pressure produces a higher probability of collision because the particle has a greater distance over which a collision can occur. This provides a direct analytical connection between chamber geometry and pressure-dependent transport.

The Knudsen-number representation of Fig. 5 provides a compact regime map. Because $Kn = \lambda/L \propto T/(pL)$, pressure, temperature and chamber distance enter through the same dimensionless transport parameter, and the transition near $Kn = 1$ is therefore

**Fig. 4:** Probability of at least one collision versus pressure for three illustrative target-to-substrate distances at 300 K, calculated from Eq. (3).

useful for organizing pressure-dependent trajectory behaviour.

3.1 Quantitative anchor values

Figures 1–5 display the pressure and temperature dependence of λ , P_{coll} and Kn continuously. Table 4 lists

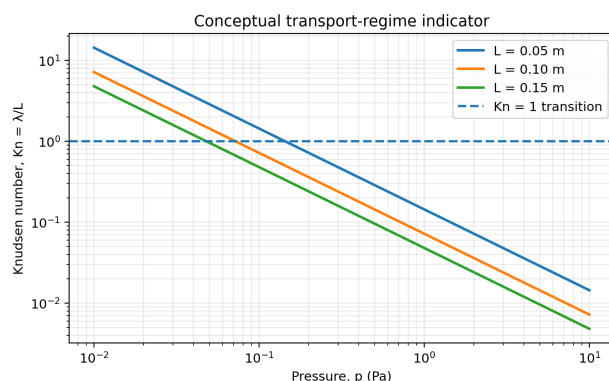


Fig. 5: Knudsen number versus pressure for three illustrative target-to-substrate distances at 300 K. The dashed line marks $Kn = 1$, separating predominantly ballistic transport ($Kn > 1$) from collision-dominated transport ($Kn < 1$).

Table 4: Anchor values of λ , P_{coll} , $\langle N \rangle$ and Kn at $T = 300$ K, $d = 0.36$ nm and $L = 0.10$ m.

p (Pa)	λ (mm)	P_{coll} (%)	$\langle N \rangle = L/\lambda$	$Kn = \lambda/L$
0.1	71.9	75.1	1.39	0.719
0.5	14.4	99.9	6.95	0.144
1	7.19	>99.99	13.90	0.0719
2	3.60	>99.99	27.80	0.0360
5	1.44	>99.99	69.51	0.0144
10	0.72	>99.99	139.02	0.00719

discrete anchor values over the pressure range of interest, calculated from Eqs. (2), (3) and (6) at $T = 300$ K, $d = 0.36$ nm and $L = 0.10$ m, so that the logarithmic trends of Figs. 1–5 can be read numerically.

3.2 Mean collision number and ballistic survival fraction

The collision probability of Eq. (3) saturates toward 100% once Kn falls below about 0.1 (Fig. 4 and Table 4), after which it no longer distinguishes mildly from heavily collisional conditions. The mean collision number of Eq. (6) and the survival fraction of Eq. (5) remain informative deep into the collision-dominated regime and are shown in Figs. 6 and 7.

The mean collision number in Fig. 6 grows as a straight line on log-log axes, directly reflecting $\lambda \propto 1/p$. At $p = 10$ Pa an atom launched over $L = 0.10$ m experiences on the order of 10^2 collisions on average, consistent with the near-unity collision probability in Fig. 4 and Table 4.

Figure 7 is the direct complement of Fig. 4 ($S = 1 - P_{\text{coll}}$) but is plotted on a scale that resolves how quickly the ballistic fraction collapses: for $L = 0.10$ m at

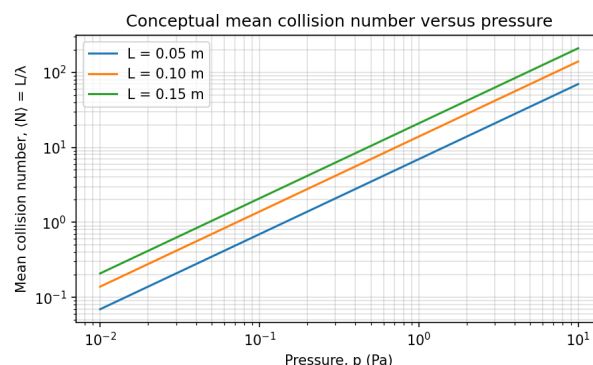


Fig. 6: Mean collision number $\langle N \rangle = L/\lambda$ versus pressure for three illustrative target-to-substrate distances at $T = 300$ K and $d = 0.36$ nm, calculated from Eq. (6).

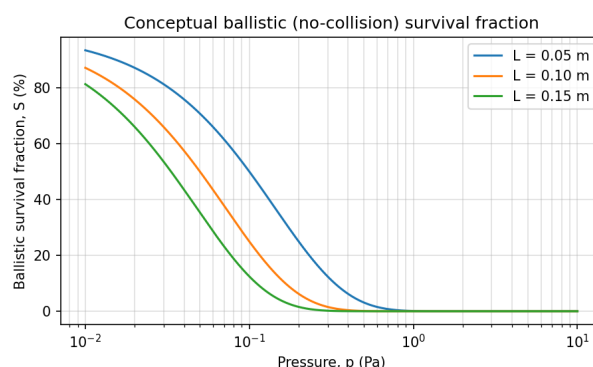


Fig. 7: Ballistic (no-collision) survival fraction $S = \exp(-L/\lambda)$ versus pressure under the same conditions as Fig. 6, calculated from Eq. (5).

$T = 300$ K the uncollided fraction falls below 1% at $p \approx 0.33$ Pa, well inside the pressure range typically used in magnetron sputtering.

3.3 Two-dimensional pressure-temperature map

Figures 1 and 3 show $\lambda(p)$ at fixed T , with the temperature dependence represented only by a discrete family of curves. Figure 8 combines both dependences in a single contour map, which is convenient for locating an operating point in (p, T) space.

The near-vertical contours show that, over the 300–450 K interval, pressure remains the dominant control variable: because $\lambda \propto T/p$, a given λ contour shifts in pressure only by the factor $450/300 = 1.5$ across the full 150 K temperature span. Temperature effects on sputtered films over a comparable range have been examined in the author's earlier work [8, 15].

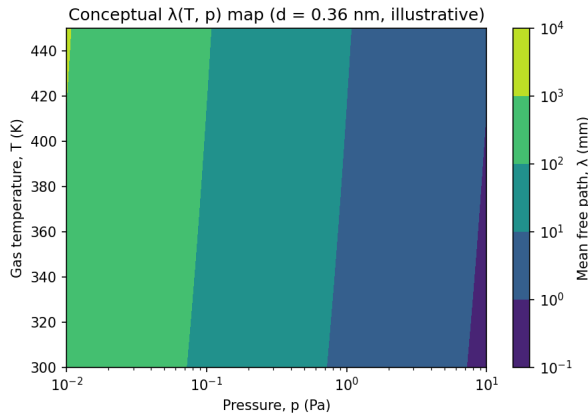


Fig. 8: Contour map of the mean free path $\lambda(T, p)$ calculated from Eq. (2) with $d = 0.36$ nm (logarithmic colour scale).

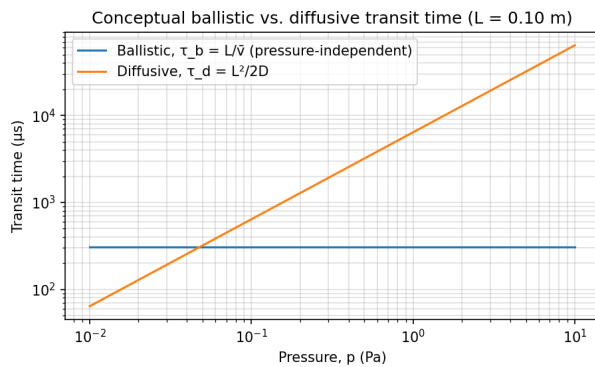


Fig. 9: Ballistic transit time τ_b (Eq. 9) and diffusive transit time τ_d (Eq. 10) versus pressure for $L = 0.10$ m, $T = 300$ K and $M = 60$ u.

3.4 Ballistic and diffusive transit times

Section 2.5 introduced ballistic and diffusive estimates of the transit time. Figure 9 compares Eqs. (9) and (10) over the same pressure range as Figs. 1–8, using $M = 60$ u, $T = 300$ K and $L = 0.10$ m.

Because τ_b is independent of pressure while $\tau_d \propto p$, the two curves cross at $p \approx 0.05$ Pa, where $Kn = 1.5$, close to the $Kn \approx 1$ condition in Fig. 5. This gives an independent, time-domain confirmation of the ballistic-to-diffusive transition identified through the Knudsen number. Table 5 lists both transit-time estimates at the anchor pressures of Table 4, together with the corresponding regime from Table 3.

Table 5: Ballistic and diffusive transit-time estimates at $T = 300$ K, $L = 0.10$ m and $M = 60$ u.

p (Pa)	τ_b (μ s)	τ_d (μ s)	Regime (Table 3)
0.1	307	641	Transitional
0.5	307	3200	Transitional
1	307	6410	Continuum
2	307	12800	Continuum
5	307	32000	Continuum
10	307	64100	Continuum

3.5 Two-stage simulation workflow

Figure 10 summarizes the two-stage SRIM–SIMTRA workflow. SRIM provides the ion–solid sputtering stage and the initial characteristics of the ejected atoms, whereas SIMTRA describes transport through the background gas and the resulting population arriving at the substrate; the transport stage is governed, to first order, by Eqs. (2) and (3) [5,6].

3.6 Scope and assumptions

The analytical transport relations are first-order kinetic-theory estimates. They assume an ideal dilute background gas, an effective collision diameter and a representative flight distance. The diffusion estimate $D = \lambda \bar{v}/3$ is a continuum-limit approximation and should not be interpreted as a substitute for a full stochastic SIMTRA trajectory calculation. Likewise, the analytical figures and anchor tables follow from the assumptions stated in this paper and do not replace detailed SRIM/SIMTRA simulation output [2,6].

4 Results and discussion

The present analysis treats deposition as a two-stage process that couples sputtering-yield characterization with gas-phase transport. This distinction is physically important: the sputtering yield determines how many particles are produced at the target, whereas pressure-dependent transport determines how the emitted population is redistributed before it reaches the substrate. SRIM and SIMTRA are complementary tools for these two stages [1, 5, 6], and the link between the sputtered-atom flux and the quality of the deposited film has been addressed in earlier work [16, 17].

The target/projectile combinations considered here span light and heavy incident species and several technologically important target elements, a matrix that is useful for examining how ion–target mass relationships affect sputtering, including for thin-film materials used in photovoltaic applications [18]. Numerical yield values, incident energies and individual SRIM output tables are

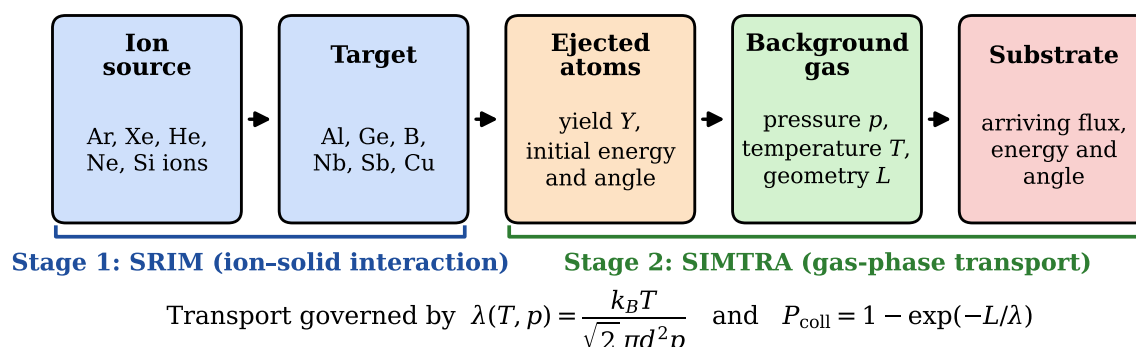


Fig. 10: Schematic of the two-stage SRIM (ion–solid interaction) and SIMTRA (gas-phase transport) workflow. The transport stage is governed by Eqs. (2) and (3).

outside the scope of the present paper, so no quantitative yield ranking is drawn from it.

For transport, the principal analytical prediction is direct: increasing pressure shortens the mean free path and increases the expected number of gas-phase collisions. In detailed particle-transport calculations, these collisions broaden the angular distribution and reduce the energy retained by sputtered atoms, and published Monte Carlo studies report pressure- and distance-dependent changes in the energy and angular distributions of the arriving particles [6, 7, 11, 12]. The anchor values in Table 4 quantify this dependence for the illustrative parameters used here: at $T = 300$ K, the transport passes from the transitional into the continuum regime of Table 3 at about 1 Pa.

Calculations over the 300–450 K interval have been compared with previous work [8]. The analytical treatment presented here complements that comparison by giving a direct physical interpretation of the pressure dependence through the mean free path and the collision probability. Because the figures in this paper are generated from analytical relations with stated illustrative parameters, they should be read as a guide to the governing physics rather than as a numerical transport dataset.

5 Conclusions

A compact SRIM–SIMTRA framework has been presented for analysing the path of sputtered atoms during thin-film deposition. SRIM characterizes atom production at the target, while SIMTRA follows the emitted population through the background gas toward the substrate.

Pressure modifies the trajectory primarily through the mean free path, while temperature and the target-to-substrate distance enter through the same

dimensionless transport parameter, the Knudsen number. The relation $\lambda \propto T/p$ shows that increasing pressure shortens the collision-free path, and $P_{\text{coll}} = 1 - \exp(-L/\lambda)$ shows that the probability of at least one collision increases for a fixed flight distance. These changes are associated with angular scattering and energy redistribution before deposition. Beyond these two relations, the paper derives complementary survival-fraction, mean-collision-number, diffusion-coefficient and transit-time expressions (Eqs. 5–10), shows that the ballistic and diffusive transit times cross at $Kn = 1.5$, and organizes the assumptions into a nomenclature table and a Knudsen-number regime classification (Tables 2 and 3), together with a two-dimensional $\lambda(T, p)$ map and a workflow schematic (Figs. 8 and 10).

The analysis considers Al, Ge, B, Nb, Sb and Cu targets bombarded by Ar, Xe, He, Ne and Si ions over the 300–450 K interval. Future work will use the full SRIM/SIMTRA output to report sputtering-yield tables, pressure-dependent arriving-atom distributions, energy spectra and deposition profiles, allowing the analytical trends presented here to be tested directly against numerical transport calculations [10].

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