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# Monte Carlo Simulations of Elastic Scattering with Applications to DC and High Power Pulsed Magnetron Sputtering for $Ti_3SiC_2$

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**Abstract.** We simulate the particle transport in a thin film deposition process made by PVD (physical vapor deposition) and present several models for projectile and target collisions in order to compute the mean free path and the differential cross section (angular distribution of scattered projectiles) of the scattering process. A detailed description of collision models is of the highest importance in Monte Carlo simulations of high power impulse magnetron sputtering and DC sputtering. We derive an equation for the mean free path for arbitrary interactions (cross sections) that includes the relative velocity between the particles. We apply our results to two major interaction models: hard sphere interaction & screened Coulomb interaction. Both types of interaction separate DC sputtering from HIPIMS.

**AMS subject classifications**: 80M31, 60J20, 65N74, 65C05, 65C35, 65C40

**Key words**: DC sputtering, MAX-phases, mean free path, particle in cell Monte Carlo collisions, Monte Carlo Markov chain.

## 1 Introduction

The main reason for studying the collision processes of elastic scattering is the need for a reliable physical description of the interactions between ions and a plasma (background gas) in high power pulsed magnetron sputtering processes for the creation of uniform, stoichiometric thin films. MAX-phases experienced a renaissance in the mid 1990s, when

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Barsoum synthesized relatively phase-pure samples of the MAX-phase $Ti_3SiC_2$, and discovered a material with a unique combination of metallic and ceramic properties: it exhibited high electrical and thermal conductivity, and it was extremely resistant to oxidation and thermal shock, and so is very attractive for industrial applications like proton exchange fuel cells (PEFC). These stoichiometries (MAX-phases) are described by the general formula $M_{n+1}AX_n$, where M is an early transition metal (Sc, Ti, V, Cr, Zr, Nb, Mo, Hf, Ta), A is an A-group element (Al, Si, P, S, Ga, Ge, As, Cd, In, Sn, Ti, Pb), and X is either Carbon and/or Nitrogen. The different MAX stoichiometries are often referred to as 211 ($n=1$), 312 ($n=2$). Recent developments have led to a new method of synthesizing thin films of MAX-phases on a substrate (workpiece): high power impulse magnetron sputtering (HIPIMS or HPPMS), see [1–4]. The most important ingredient in sputtering processes is a plasma, i.e., a partially ionized gas, which, at macroscopic scales, is electrically neutral. If a material body such as a substrate is immersed in a plasma it will acquire a potential slightly negative with respect to ground. This effect is known as a floating potential. The physical reason for this is the higher mobility of electrons than that of ions. Hence, more electrons reach the substrate surface than ions. A very sensitive quantity in sputtering processes (with respect to the experimental setup: gas-pressure, temperature, target-material, etc.) is the sputtering yield, which describes the ratio of atoms ejected from a target surface per incident ion. The sputtering yield can take almost any value from 0.1 up to 10. To optimize production, one is generally interested in obtaining values for the sputtering yield as high as possible. In order to obtain a well defined film stoichiometry at the substrate, one has to take into account the transport mechanism of the sputtered particles within the plasma. This can be done either within a macroscopic description of the transport phenomena, i.e., the solution of the advection–diffusion equation, or at a microscopic scale, via Monte Carlo simulations of the transport phenomena. This paper deals almost exclusively with the last approach, in the future, the ultimate goal of our work will be to link both approaches to each other (this will be presented in future papers).

This paper is organized as follows: In Section 2 we describe the concept of mean free path and derive, on the basis of the kinetic theory, an appropriate expression for the mean free path of an external particle (projectile) that is probing an ensemble of target particles that constitute an ideal gas (background gas). The main modification to standard mean free paths is to allow of initially moving targets. Section 3 studies, from first principles, the concept of differential cross sections. In Section 4 we present our Monte Carlo method based on a pathway model, see [5], and perform several simulations of direct current (DC) and high power pulsed magnetron sputtering (HIPIMS). At the end, in Section 5, we summarize our results and discuss perspectives for future work.

## 2 Collision model: mean free path

The mean free path or average distance between collisions for a gas molecule may be estimated from kinetic theory. If one assumes the gas consists of hard spheres (non over-