Nuclear Inst. and Methods in Physics Research B 420 (2018) 27–32

Contents lists available at ScienceDirect

Nuclear Inst. and Methods in Physics Research B

journal homepage: www.elsevier.com/locate/nimb

A model for sputtering from solid surfaces bombarded by energetic clusters

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ARTICLE INFO

Keywords:
Sputtering
Cluster
Nanoparticle
Shock wave
Model

ABSTRACT

A model is developed to explain and predict the sputtering from solid surfaces bombarded by energetic clusters, on the basis of shock wave generated at the impact of cluster. Under the shock compression the temperature increases causing the vaporization of material that requires an internal energy behind the shock, at least, of about twice the cohesive energy of target. The sputtering is treated as a gas of vaporized particles from a hemispherical volume behind the shock front. The sputter yield per cluster atoms is given as a universal function depending on the ratio of target to cluster atomic density and the ratio of cluster velocity to the velocity calculated on the basis of an internal energy equals about twice cohesive energy. The predictions of the model for self sputter yield of copper, gold, tungsten and of silver bombarded by C_{60} clusters agree well, with the corresponding data simulated by molecular dynamics.

1. Introduction

In recent times, the clusters used as projectiles have attained importance specially in connection with sputtering and the depth profiling. These projectiles are currently receiving broad scientific interest due to their capability in sputtering from solid surface. Although, their interaction with surface remains a very complex problem which has challenged theoretical and experimental investigators for quite some time, there exist some approaches to study the sputter yield, and the depth profiling. More recently, several formulas have been proposed in an attempt to approximate the measured and simulated sputter yield, based on molecular dynamics simulations [1] or modelling of experimental data using purely empirical relationships [2–4]. Indeed, sputtering of a condensed-gas solid induced by the impact of atomic clusters (sizes $n \leqslant 10^4$) has been studied by molecular dynamics simulation [2]. The authors found that the sputter yield can only depend on the projectile cluster size n and the scaled total energy E/u_0, where u_0 is the binding energy of the target material. In addition, they obtained a formula that contains three unknown parameters namely α, b and ϵ_c (threshold energy), which are fitting parameters. Sputtering yields of materials for argon cluster ions used in SIMS and XPS has, also, been analysed [4] as a function of cluster size and energy in the range from 2.5 to 80 keV. Accordingly, the sputtering yield has been described by a formula involving two unknown parameters A and q which depend on the cluster size n and its energy E. Until now, the first analytical description of the sputter yield assuming a Gaussian distribution of deposited energy by the cluster was that developed in reference [5] to obtain an equation for estimating the sputter yield by fitting three parameters to experimental data. In fact, the aforementioned approaches work as mathematical formula including for experimental planning and quantification of depth profiles for studied materials, but they provide no information with regard to physical mechanism behind the sputtering under impact of a large clusters or nanoparticles.

It is important to note that sputtering under impact of atomic ions has been widely studied theoretically to explain the emission of intact molecules in the gas phase from organic surfaces at high energy density. Moreover, the idea of collective emission was introduced initially as a new basis in some analytical models to describe the mechanism of emission in terms of gas-flow [6], shock wave [7–9], pressure pulse [10,11] and thermal spike based on the fluid dynamics calculations [12]. However, a comparison between atomic impacts and cluster impacts seems to be difficult even at equal velocity. Indeed, unlike atomic ion, a cluster is a unique tool for bombarding small area of a solid by several atoms simultaneously and for depositing large energy densities in the solid inducing nonlinear collective effects [13].

The purpose of this article is to study the physical process by which the energy deposited in the atomic system will be converted into collective motion of atoms leading to sputtering from the surface. For this end, we propose a model based on the shock wave generated upon impact of cluster on the surface to explain the expression of sputter yield per cluster atoms known as universal representation. After presentation of the model in Section 2, the analytical predictions of model will be discussed and compared in Section 3with some simulated data by molecular dynamics method. A general conclusion will be given in Section 4.

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https://doi.org/10.1016/j.nimb.2018.01.030
Received 18 December 2017; Received in revised form 24 January 2018; Accepted 25 January 2018

List of symbols

Cluster	
m_1	atomic mass of cluster constituents
n	size of cluster projectile ($n = n_p \Omega_c$)
n_p	atomic density of cluster-projectile
r_0	radius of spherical cluster
R_{WS}	Wigner–Seitz radius $\left(R_{WS} = \left(\frac{3m_1}{4\pi\rho_1}\right)^{1/3}\right)$
u_1	particle velocity behind shock wave in the cluster
v_i	impact velocity of cluster(incident velocity)
ρ_1	density of cluster material
Ω_c	volume of cluster $\left(\Omega_c = \frac{4\pi}{3} r_0^3\right)$
Target	
c_0	speed of sound at zero pressure
ΔH_s	heat of sublimation
m	mass of target atom
n_t	atomic density of target
p	pressure behind shock wave $p = \rho_0 w\, u$
r	radius of contact between the cluster circumference and the target surface
$\dot{r}$	collision point velocity on the target surface
s	slope parameter in the linear equation $w = c_0 + s\, u$
u	particle velocity behind the shock front
u_0	energy of sublimation (or cohesive energy)
$\bar{v}$	mean velocity of particle flux defined as $\bar{v} = \sqrt{\frac{4u_0}{m_2}}$
w	velocity of shock wave
x	lowest position of cluster with respect the free surface $(x,0)$
ϵ	specific internal energy behind shock wave
η	ratio of density ρ_0 to density ρ behind shock wave $(\eta = \rho_0/\rho)$
ϑ	angle between the tangent to the cluster at collision point and target surface
ξ	parameter of proportionality in equation $\epsilon = \xi\, u_0$, where $\xi = \frac{1}{f\, m} \frac{(s\,\eta)^2}{(1-(s\,\eta))^2}$
	a function of angle ϑ, that is $\omega = 1 - \frac{1}{\sqrt{1 + tan^2(\vartheta)}}$

2. Theoretical model

In spite of the complexities involved with the cluster impact process, some simplified assumptions can be made to analytically treat the problem. For this purpose, we consider a spherical cluster of size n, a radius r_0, normally impacting on a planar solid surface with supersonic velocity v_i. In the beginning of penetration process, the 'edge atoms' of cluster push the target atoms around the impact point that become extensively displaced [14] and a vast disordered region is formed [15] resulting in a shock wave formation. In fact, generation of shock wave upon impact of energetic cluster has been revealed by molecular dynamics simulation in a diamond target impacted by Co_n and Ar_n clusters [16] and in molybdenum surface impacted by Mo_{1043} clusters [17]. This shock wave propagates into the target and backward into the cluster compressing the material that they pass through.

We consider the general case where the materials of cluster and target are different. For this end, the quantities describing shock wave in the cluster projectile are noted by the subscript 1 and the quantities for the target are without subscript, except the usual parameters (ρ_0, c_0 , ϵ_0 , T_0 and p_0).

The shock front moves through the sample with a velocity w while the material particles behind shock front move with a velocity u. The shock causes the passage of target material from an initial state (p_0, ρ_0 , ϵ_0) to a new state (p, ρ , ϵ) that is characterized by high pressure and high temperature along the Hugoniot curve causing the specific internal energy to increase. The pressure p, the density ρ, the change in the target internal energy $\epsilon - \epsilon_0$ and the velocities w and u, are determined by mass, momentum and energy conservation laws across the shock front in the frame of un-shocked matter [18] in the Appendix.

We consider the impact point of cluster on the surface as origin of a coordinate system *xoy* in which x axis is directed inwards in the direction of impact velocity and y axis is tangent on the surface perpendicularly to x axis as illustrated in Fig. 1. The impact of spherical cluster on the surface is characterized by a circumference of radius r that depends on the cluster radius r_0 and its lowest position $x$with respect to the target surface, that is

$$r^2 = (2r_0 - x)x \tag{1}$$

where $r_0 = R_{WS}\, n^{1/3}$, and $R_{WS} = \left(\frac{3m_1}{4\pi\rho_1}\right)^{1/3}$ is the Wigner–Seitz radius.

Differentiating Eq. (1) with respect time yields the collision point velocity $\dot{r}$ on the target surface [19]

$$\dot{r} = \frac{(r_0 - x)v_i}{\sqrt{r_0^2 - (r_0 - x)^2}} \tag{2}$$

The target material in the region between the incoming cluster and the target, is shocked by the cluster and therefore may be removed during the impact, in the form of jetting [19–21]. In addition, the onset of jetting observed when two thin plates collide creating a jet, has been extended to the impact of a spherical projectile into a flat target [20]. In fact, ejection of particles from a shocked region begins when the condition $w \geqslant \dot{r}$ becomes satisfied [19]. This condition ensures that the shock wave detaches from the collision point allowing for rarefaction waves to propagate into the shocked material inducing collective ejection of particles. It has been demonstrated that, when the shock wave reaches the interface between the surface and a vacuum the material begins to expand from the surface [22]. one way to apply this condition would be to consider the equality [23] $w = \dot{r}$, which leads to $x = r_0(1 \pm w/\sqrt{w^2 + v_i^2})$ or simply $x = r_0\,\omega$, where is a function defined so that, for $v_i = 0$ there is no penetration in the target that is $x = 0$,

$$\omega = 1 - \frac{w}{\sqrt{w^2 + v_i^2}} \tag{3}$$

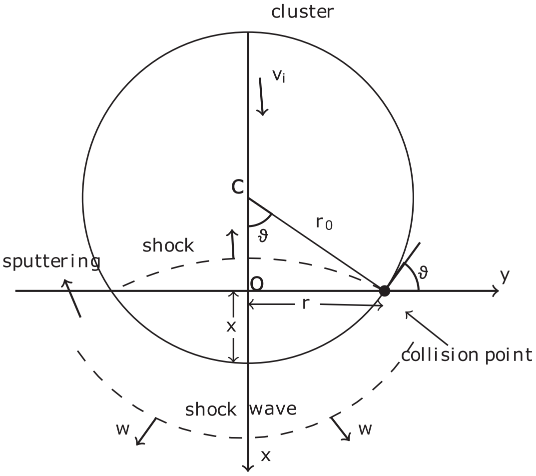

Fig. 1. Schematic view of penetration process of a spherical cluster of radius r_0 normally impacting a flat surface. r is the radius of contact area between cluster and target surface and x is the lowest position of cluster below the surface. The elliptic dotted surfaces are the shock waves generated in the projectile and target.