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Monte Carlo simulations of MgO and $Mg(OH)_2$ thin films sputtering yields by noble-gas ion bombardment in plasma display panel PDP

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ABSTRACT

MgO is known to be a material suitable for barrier coating of commercial plasma display panel (PDP) cells owing to its excellent electrical insulating property, good resistance to sputtering, large secondary-electron emission coefficient and high transmittance. It is also a valuable information for improving the efficiency and the lifespan of the PDP. However, the effect of moisture emitted from the wall and phosphor materials of the PDP cells, an $Mg(OH)_2$ is formed on the top surface of an MgO protective layer. In this work, the Monte Carlo simulation program SRIM-2013 was applied to calculate the sputtering yields of magnesium hydroxide $Mg(OH)_2$ by low-energy noble-gas ion bombardment. The comparison between results obtained by Monte Carlo simulation and those obtained by experiments is elucidated in this paper. Furthermore, the surface binding energies for MgO and $Mg(OH)_2$ layers on sputtering yield are discussed. It is found that the sputtering yield of $Mg(OH)_2$ is generally lower than that of MgO at each incident energy. On the other hand, the sputtering yield depends on the properties of both the incident particle and the target.

1. Introduction

In 1852, W. R. Grove first discovered the sputtering phenomenon, which is driven by the physical removal of atoms from a solid surface by incident energetic particle bombardment in a dc gas discharge tube. Physical sputtering is a consequence of energy and momentum transfer between the incident ions and the target atoms, due to collisions [1,2]. It is characterized by the sputtering yield, i.e. the mean number of released atoms per incident particle [3] depends on the ion incident energy, the ion incident angle, the surface binding energy, the masses of the ion and target atoms, but it is independent of the charge. A surface atom may be ejected as a sputtered particle if the incident ions establish collision cascades recoil and reach the target surface with an energy greater than the surface binding energy. The threshold energy E_{th} is defined as the minimum kinetic energy required below which the sputtering yield is zero [4]. The sputtering is commonly developed and used for thin-film deposition, analytical techniques, surface cleaning and etching [5]. This process is regarded as undesired side effect such as in the reactor ITER [6], fluorescent lamp and plasma display panel (PDP). The most important element causing the degradation of the cell and limiting the lifetime of the PDP is the sputtering of the MgO layer by energetic ions and fast neutrals. This layer is deposited above the dielectric film covering the cathode electrodes [7]. In particular, sputtering of the protective layer in PDP depends not only on the property of the protecting layer, but also on the condition of the inert gas mixture. In commercial PDP cells, magnesium oxide (MgO) plays an extremely important role in protecting the dielectric layer from plasma damage and keeping the operating voltage relatively low owing to its high sputter resistance, excellent electrical insulating property, large secondary-electron emission coefficient and high transmittance [8]. In addition, the effect of moisture inadvertently emitted from the wall and phosphor materials of the PDP cell may hydrate the top surface of MgO barrier coat to form a thin layer of magnesium hydroxide $Mg(OH)_2$. The chemical equation below describes the exothermic hydration reaction of MgO [9]:

$$Mgo(s) + H_2O(g) \rightarrow Mg(OH)_2(s)$$

Thus, hydration is one of the critical problems of MgO protective layer for the PDP, since it reduces the secondary electron emission coefficient and increases the sputtering yield of the barrier coat, which increases the discharge voltage [10]. Many articles have been written on the sputtering yield and lifetime of PDPs. We can mention here, for instance, experimentally obtained CaO, SrO and BaO sputtering yields for He, Ne, Ar, Kr and Xe ion injections have been represented in Refs [11,12]. Other experimentally measured sputtering yields of MgO and $Mg(OH)_2$ by low-energy noble-gas ion bombardment have also been reported in Refs. [9,13,14]. On the theoretical sides, Yoon et al. [15] reported the calculated sputtering yield of the MgO by using numerical

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simulations based on a binary collisions model. Similarly, Piscitelli et al. [16] also calculated the erosion rate of Ne and Xe on MgO by using hybrid simulation method. In Ref [17], Molecular Dynamics simulations were performed on the sputtering properties of MgO surface by He, Ne and Xe.

As far as we know, the Monte Carlo simulations of $Mg(OH)_2$ sputtering yields by noble-gas ion bombardment and those of MgO by Kr ion bombardment in the low-energy range have not yet been investigated. This paper is devoted to this point.

It is known that the Monte Carlo method is a very feasible way to calculate the trajectory of the incident ion and the damage produced by that ion in materials based on the binary collision approximation model [18]. Stopping and Range of Ions in Matter, or SRIM (formerly TRIM) is a group of computer programs which calculate many features of the transport of ions in matter using a quantum mechanical treatment of ion-atom collisions , such as target damage, sputtering yield, ionization, implantation and phonon production [18]. It is based on Sigmund's theory of physical sputtering [26]. This program considers only binary collisions with target atoms initially at rest.

The goal of this research is to show that the surface binding energy of both MgO and $Mg(OH)_2$ changes due to the bombardment of (He, Ne, Ar, Kr and Xe) incident particles. In addition, to evaluate the influence of the mass density on the sputtering yield (inversely proportional to the lifetime [7,15]) of MgO layer in the PDP.

The article is structured as follows. In Section 2, we present Sigmund's theory of physical sputtering. In Section 3, we provide the background information about the interatomic potential and the simulation model used here, and we describe the computational methodology. The obtained results are compared with experimental data by Ikuse et al.[9], and numerical simulation data of MgO obtained previously [15]. Thus, our results are presented and discussed in Section 4. Finally, our conclusions are given in Section 5.

2. Sputtering theory

The sputtering yield (SY) is an essential parameter to assess the quantity of ejected atoms under ion bombardment, as stated in Eq. (1):

$$SY = \frac{\text{number of ejected target species (Ne)}}{\text{number of incident ions (Ni)}} \tag{1}$$

Sigmund assumption of linear collision cascades theory is developed for amorphous targets in solving the Boltzmann transport equations [20]. This theory is used to calculate the sputtering yield, as in the following expression [19] $SY(E_0, \theta_0) = \Lambda E_D(x=0, E_0, \theta_0)$, where Λ is the material factor, which reflects the range of displaced atoms, the number of atoms ejected and the surface binding energy. The energy deposition is expressed by the numerical calculation given as [19] $E_D(x=0, E_0, \theta_0) = \alpha N S_n(E_0)$, in which N is the atomic density of the target, $S_n(E_0)$ is the nuclear stopping cross section, x is the depth of the particles in the target and α is a numerical factor depending on the initial angle of incidence θ_0 and the mass ratio between target and projectile M_2/M_1 [20]:

$$\alpha = \begin{cases} \sim 0,\ 2 & \text{for } \frac{M_2}{M_1} \leqslant 0.5 \\ 0.3\left(\frac{M_2}{M_1}\right)^{2/3} & \text{for } 0.5 < \frac{M_2}{M_1} \leqslant 10 \end{cases} \tag{2}$$

Thus, the nuclear stopping cross section $S_n(E_0)$ is written [19]:

$$S_n(E_0) = \frac{8.462\, Z_1 Z_2 S_n(\varepsilon)}{(1 + M_2/M_1)(Z_1^{0.23} + Z_2^{0.23})} [10^{-15}\text{ev. cm}^2] \tag{3}$$

where $Z_1$and $Z_2$are the atomic numbers for each of the incident particle and material target respectively, and $S_n(\varepsilon)$ is the reduction of nuclear cross section, it is expressed by [19]:

$$S_n(\varepsilon) = \frac{0.5 \ln(1 + 1383\varepsilon)}{\varepsilon + 0.0132\varepsilon^{0.21226} + 0.19593\varepsilon^{0.5}} \tag{4}$$

The reduced energy ε is given by the following equation [19]:

$$\varepsilon = \frac{32.53\, M_2 E}{Z_1 Z_2 (M_1 + M_2)(Z_1^{0.23} + Z_2^{0.23})} \tag{5}$$

3. Monte Carlo simulations

3.1. Interatomic potential

Based on the Monte Carlo simulation program SRIM that uses the binary collision approximation (BCA), applied to ion-solid interactions. the universal potential or Ziegler-Biersack-Littmark (ZBL) potential is given by [21] $V_{ZBL}(r) = \frac{Z_1 Z_2 e^2}{4\pi\varepsilon_0 r}\phi\left(\frac{r}{a}\right)$,where $Z_1$and $Z_2$are the atomic numbers of the incident ion and the target atoms respectively, $\varepsilon_0$is the permittivity of free space, r is the interatomic distance, e is the electronic charge, $A_i$and $B_i$are fitting parameters, a is an empirical screening length.

The universal screening function $\phi\left(\frac{r}{a}\right)$ expressed as [17]:

$$\phi\left(\frac{r}{a}\right) = \sum_{i=1}^{4} A_i e^{-B_i \frac{r}{a}} \tag{6}$$

$$= 0.1818\, e^{-3.2\frac{r}{a}} + 0.5099 e^{-0.9423\frac{r}{a}} + 0.2802 e^{-0.4029\frac{r}{a}} + 0.02817 e^{-0.2016\frac{r}{a}} \tag{7}$$

This function is determined by exact fitting of the calculated interatomic potentials of 522 randomly chosen pairs of atoms. In addition, the screening length depends on the atomic numbers (Z_1, Z_2) and the Bohr radius (a_0) by semi-empirical formula [21] $a = \frac{0.8854 a_0}{Z_1^{0.23} + Z_2^{0.23}}$, where $a_0 = 0.529$ Å.

3.2. Calculation details

The software package SRIM-2013 proposed by J.F Ziegler and J.P Biersack [27], which is one of the most computer programs simulating the sputtering process, because of its extensive database on compound target materials and its convenient user interface [28]. In order to study the sputtering effects of targets by focused ion beams, Monte Carlo simulations code SRIM-2013 of ions impacting (He, Ne, Ar, Kr and Xe) on magnesium hydroxide $Mg(OH)_2$ substrate were carried out in the energy range 26–300 eV, the angle of incidence for all ion beams was normal to the substrate surface. As a result, in our calculations, the Mg $(OH)_2$ can be thought as an amorphous material or random solid when considering its sputtering yield, which equals to the sum of sputtering yields of Mg, O and H atoms. Hence, there is no effect of sample crystallinity on the measured sputtering yields. This simulation method has been previously used to study the sputtering yields of MgO [15]. The input parameters for the simulations are summarized below:

In Table 1, we report the SRIM input parameters required for sputtering calculations include the total number of incident projectiles and the composition of the two layers MgO and $Mg(OH)_2$. According to this Table 1, we see that the total number of primary ions impacting on each layer in the simulation was 100,000 [29] in order to obtain better statistical values and to avoid higher fluctuations, because the

Table 1
Parameters input used in calculating the sputtering yields of the two layers MgO and $Mg(OH)_2$.

	MgO		$Mg(OH)_2$		
Total number of ions	100,000		100,000		
Mass density (g/cm^3)	3.4		2.4		
Thickness (Å)	10,000		2000		
Surface binding energy (eV)	Mg: 10	O: 10	Mg: 10	O: 10	H: 10
Lattice binding energy (eV)	Mg: 3	O: 3	Mg: 3	O: 3	H: 3
Displacement energy (eV)	Mg: 25	O: 28	Mg: 25	O: 28	H: 10