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Dependence on size and curvature of sputtering yield in nanowires

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ABSTRACT

Bombardment of different <110> Co nanowires with 1-k eV argon ions along a <100> direction is simulated by molecular dynamics. Sputtering yield is analysed for different surface curvatures. For that purpose, results on three cross-section shapes were obtained, namely: circular, square and rhomboid. A low dose is used to avoid great surface damage. Yield increases with increasing curvature. However, if the cross-section size decreases, this dependence is modified and other phenomena such as spike sputtering occur. In particular, this effect causes an abundant sputtering. The Sigmund theoretical model was used to compare predictions. Results for sputtering yield show a maximum and an asymptotic behaviour for large nanowire sizes. These asymptotic values confirm the dependence on curvature. This dependence for small sizes differs from the simulation model. The Sigmund model does not take into account the local heating, besides it assumes that the energy deposition profile does not depend on target size. The angular distributions of the speed vector show that the lattice structure determines the directions of ejection, and therefore, this structure would also influence the sputtering yield.

1. Introduction

Ion implantation is a technique to insert atoms in the form of ions into a target material. The objective is to dope this material or to tune its properties by generating defects or modifying its composition [1]. When ion irradiation occurs, another important effect takes place: sputtering, that is, the ejection of atoms from the surface due to the collisions with energetic particles.

The Sigmund model [2] is nowadays the most widely accepted model for estimating sputter yield, i.e. the mean number of atoms ejected per incident ion. The dependence of sputtering yield on bulk properties of the target is described reasonably well by this model which is originally circumscribed to linear effects and amorphous targets [3]. The interest in sputtering of nanoparticles and nanostructured surfaces is currently increasingly greater [4]. However, the dependence of sputtering on the actual surface topography of the target is difficult to quantify, especially in systems such as nanoislands [5,6] or nanowires [7,8] and in materials with a crystallographic structure such as metals. In these systems, the influence of cross-section shape as well as other factors, plays an important role as shown in recent works. Thus, Urbassek et al. [9] showed analytically and by simulation that the bombardment of convex surfaces produces an increase in sputtering yield. Previously, Johannes et al.[10] had demonstrated that in the bombardment of nanowires, yield attained a maximum if the ion range was similar to the nanowire diameter.

Unlike previous works, we are interested in analysing the dependence of sputter yield on curvature for small diameters, i.e. sizes in which the curvature fails to be a determinant factor. Therefore, we will highlight those phenomena that mark the transition and modify the dependence on curvature for large diameters. Co nanowires is a system with interesting magnetic applications in high-density magnetic recording devices [11]. So, we use <110>-oriented face-centred-cubic Co nanowires of different cross sections: circular, square and rhomboid- and different sizes. In all cases, the bombardment by molecular dynamics (MD) took place along a <100> direction of nanowire with Ar ions at 1 keV. In these systems, we calculated the mean sputter yield by using the Sigmund model of ion sputtering [2]. It is especially interesting to compare these results with those obtained by MD simulations. In order to briefly summarize our conclusions, we will say that the size notably influences the number of extracted atoms for low dimensions, and then the simulation and analytical results differ especially. This fact might indicate that other factors can take part in the process. The shape also affects sputtering. Our results point

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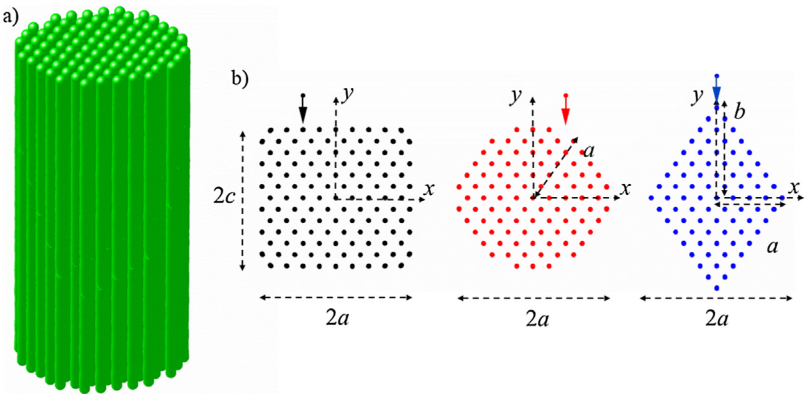

Fig. 1. (a) Perspective view of a circular cross-section nanowire (size 2). (b)*xy*-projections (cross section) of square ($c \sim a$), circular and rhomboid nanowires (size 2). The ion is also shown next to an arrow. All figures correspond to the initial state.

out that surface curvature influences the yield, the simulation and analytical results agree, especially for great dimensions.

2. Computational and analytic methods

In this work, the simulation of the bombardment of targets formed by Co nanowires with <110> orientation was accomplished by MD. Ar ions were thrown at 1 keV along a <100> direction. The second-moment tight-binding approximation (TB-SMA) potential [12] modelled the atomic Co interactions. At short distances, this potential was smoothly linked to the universal repulsive Ziegler-Biersack-Littmark (ZBL) potential [13]. This latter potential also describes the Ar-Co interactions. Besides, we considered that atoms with kinetic energy higher than 10 eV suffer inelastic energy losses. [12]. In order to find out the influence of curvature on sputtering, three cross-section shapes were used: square, circular and rhomboid. The circular cross section is maybe the most realistic since nanowires generally have a smooth outline. The other two are selected due to their extreme values of curvature. In Fig. 1(a), a 3D image of a circular-shaped nanowire is shown. In addition, five nanowire widths, $2a$, transversal to the bombardment direction were simulated (see Fig. 1(b)): $a = 6.5$ Å (size 1), $a = 11$ Å (2), $a = 18$ Å (3), $a = 25$ Å (4), $a = 32$ Å (size 5); these systems will allow us to study the dependence of sputtering yield on size.

The nanowire length was about 70 nm. At both ends, the nanowire was fixed (about 20 layers). Next to these layers, 40 layers (also placed at both sides) thermally controlled the system using the generalized Langevin equation proposed by Adelman and Doll [14]. These layers absorbed heat in order to maintain a temperature close to 5 K, and thus minimizing the influence of temperature.

In Sigmund theory [15], the sputtering yield is proportional to the energy deposited by the incoming ion on the nanowire surface, S, obtained from the damage distribution F. The yield for an ion impinging the surface at $\vec{r}_0(x_0, y_0, z_0)$ is:

$$Y(\vec{r}_0) = \Lambda \int_S dS\, F(\vec{r}, \vec{r}_0) \qquad (1)$$

where Λ remains constant. And the mean sputtering yield is obtained by averaging the yield $Y(\vec{r}_0)$ over the different impact points (surface S_0), i.e.:

$$Y = \int_{S_0} dS_0\, Y(\vec{r}_0)/S_0 \qquad (2)$$

A Gaussian approximation for the damage distribution is normally used [5,16]:

$$F(\vec{r}, \vec{r}_0) = \frac{E}{(2\pi)^{3/2}\alpha\beta^2} \exp(-\frac{1}{2\alpha^2}[y - (y_0 - d)]^2)$$
$$\exp(-\frac{1}{2\beta^2}([x - x_0]^2 + [z - z_0]^2)) \qquad (3)$$

where E is the ion energy, d is the maximum depth of the damage distribution, and α, β are the standard deviations along and across the bombardment direction respectively. Several problems arise at this point that can lead to different values of these parameters. The target is a crystalline system; hence measures for one are different than for several ions due to amorphization effects. Time and space range of measure of the energy profile should be chosen suitably. Besides, the nanowire outline can deform the distribution function. In this work, we used the following values for these quantities: $d = 3$ Å, $\alpha = 15$ Å, $\beta = 10$ Å obtained averaging results for 5 ions. The parameter Λ can be determined from some experimental value of the sputtering yield. Failing that, a simulation result can also be valid as occurs in this work. The value of Λ (0.21665 Å/eV) was obtained so that the mean sputtering yield corresponding to the simulation and the analytic results coincided for the square shape (size 3), that is, $Y = 8.3$.

3. Results and discussion

First at all, we will discuss the results of the analytical model. Eqs. (1) and (2) can be integrated numerically or analytically for the three types of chosen shapes. For the circular shape of radius a, the mean yield is obtained from cylindrical coordinates by:

$$Y(\theta_0) = \frac{E\Lambda a}{2\pi\alpha\beta} \int_0^{2\pi} d\theta \exp(-\frac{1}{2\alpha^2}\left[a(\sin\theta - \sin\theta_0) + d\right]^2)$$
$$\exp(-\frac{1}{2\beta^2}\left[a(cos\theta - cos\theta_0)\right]^2) \qquad (4)$$

$$Y = \frac{1}{\pi} \int_0^{\pi} d\theta_0 Y(\theta_0) \qquad (5)$$

where the mean value is obtained by integrating only in the angular coordinate between 0 and π since the bombardment affects only half of the nanowire surface. In the case of the rhomboid shape (a perpendicular and b parallel to the bombardment direction), the

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