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Computer simulation of multicomponent ion beam enhanced deposition of (TiMo) N films

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Abstract

A Monte Carlo computer simulation code has been developed to describe the behavior of incident particles and the growth of (TiMo) N films in the multicomponent ion beam enhanced deposition process, which combines bombardment with a multicomponent ion beam of $N^+ + Mo^+$ and sputter deposition of a Ti film. The film composition profile and intermixed layer between the substrate and the film were studied using a computer simulation method. It is shown that Mo ion implantation has a stronger mixing effect in the film–substrate interface than does N ion implantation. The N profile of the computer simulation conforms to that of the Auger electron spectroscopy results. © 1998 Elsevier Science S.A. All rights reserved.

Keywords: Computer simulation; Ion beam enhanced deposition; (TiMo)N films

1. Introduction

Ion beam enhanced deposition (IBED), which is also called ion beam assisted deposition, provides a powerful means for modifying the microstructure and properties of thin films and coatings. Technically, IBED means the bombardment of a film with a energetic particle beam during deposition. The basic motivation for development of the IBED process is the need for independent control of film composition, good adhesion of film and substrate and low substrate temperature during deposition [1]. At present, by combining evaporation or sputtering processes with ion beam implantation a variety of IBED methods have been developed. High quality films and coatings with good adhesion can be prepared using this method [2].

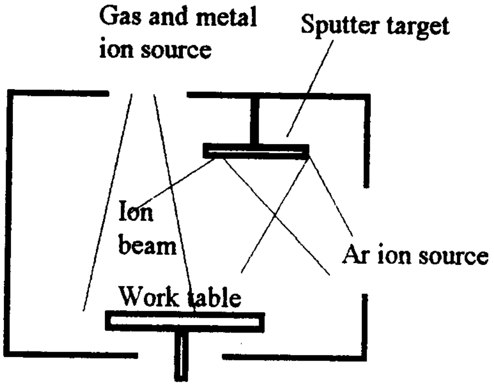

Fig. 1. The MIBED apparatus, including the all-element ion implantation system, low energy sputtering source, vacuum system and rotating water-cooled work table.

The so called all-element IBED system used here is the combination of an all-element ion implanter with an ion beam sputtering source. Its structure is shown in Fig. 1. The all-element ion implanter is capable of extracting a gas ion beam or metal ion beam simultaneously or separately with an extracting voltage of 10–80 kV. The implanter works in a pulse mode and the pulse width is 0.4 ms. This system has not only the traditional function of gas ion beam enhanced deposition, but also the new function of metal ion beam or metal plus gas IBED which is called multicomponent IBED (MIBED). In this work an N plus Mo ion beam was used to enhance the Ar ion sputter-deposited Ti film. These two processes proceeded simultaneously. The extracting voltage was 40 kV with an incident angle of 0°. The N pressure was 2×10^{-2} Pa during the

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MIBED process and the growth rate of the film was about 15 nm min^{-1}.

2. Model of calculation

Monte Carlo simulation can directly describe the collision processes of the incident ions and the target particles and is believed to be a reliable method. Many Monte Carlo computer programs have been developed to study the penetration process of incident ions in a target, such as TRIM [3], MARLOWE [4] AND EVOLVE [5]. A static target model is used for most of these computer programs. However, the static target model is not suitable in the condition of multicomponent target and high does implantation, especially the MIBED process, because (a) the target composition in the MIBED process varies continuously which changes the stopping power of the target, and (b) the surface position of the target changes continuously.

The MIBED process is a simultaneous and continuous process of implantation and deposition. To simulate the MIBED process, the implantation process and the deposition process are treated as alternative processes and the growing film is subdivided into layers which are thin enough to approximate the actual continuous process. The atoms in the film come from the implanted ions of N^+ and Mo^+, the sputter-deposited Ti and the absorbed N in the film surface. The arrival rate of Ti, N^+ and Mo^+ can be measured easily. The sputter-deposited Ti has a strong chemical activity and the time order for N_2 to cover half of the Ti surface is about 10^{-2} s in N_2 at a pressure of 10^{-2} Pa [6]. The frequency v of N_2 colliding with the Ti surface is [7]:

$$v = cp/\mu T \tag{1}$$

Here c is a constant, p is the pressure of N_2 in the chamber, μ is the molecule weight of N_2, and T is absolute temperature. The number A of nitrogen molecules adsorbed on the Ti surface is:

$$A = \alpha v \tag{2}$$

Here α is the adsorption coefficient. The arrival rate of the adsorbed nitrogen at film surface can be evaluated from Eq. (2). Then the arrival ratio of all types of particles in the deposition process can be determined.

The growing film and the substrate are subdivided into layers 4 nm thick. Pseudoparticles and pseudoprojectiles are used and each pseudoparticle or pseudoprojectile stands for 10^{14} real particles or projectiles. After a layer of Ti and adsorbed N has been deposited on the sample in the simulation procedure, the Mo ions and N ions are implanted into the sample. When the implantation is completed, the calculation begins for the new layer, and this pattern is repeated until the whole film calculation is completed.

The Mo ion beam and N ion beam are in a multicharged state, with the ratios $Mo^+:Mo^{2+}:Mo^{3+}:Mo^{4+} = 2:6:3:1$ and $N^+:N_2^+ = 2:1$. So the implantation of each layer contains ions of different charge states. The thickness and composition of each layer are adjusted after every four incident Mo pseudoprojectiles according to the number of vacancies and interstitials produced in the collision cascade, in order to make the density and the composition of each layer rational.

The fundamental model for the penetration, the sputtering and the collision cascade of the incident ion in the target as well as the principal parameters are quoted from Ref. [3]. The Bragg rule of electronic stopping is adopted for the multicomponent target. The j type of the target atoms colliding with the incident ions, related to the nuclear energy transfer, is determined by the following formula:

$$\sum_{i=1}^{j-1} C_i\sigma_i \Big/ \sum C_i\sigma_i \leq R < \sum_{i=1}^{j} C_i\sigma_i \Big/ \sum C_i\sigma_i \tag{3}$$

Here R is a random number of (0,1), σ_i is the total scattering cross-section of i type atoms colliding with the incident ion [8], and C_i is the atomic concentration of i type atoms in the film. The extracting voltage of the incident ions is 40 kV and the range of the incident ions in the target is several tens of nm. The concentration of the incident ions in the surface of the film is very low. Generally, the sputtered particles come from the target surface layer over several nm. So the probability that incident ions are sputtered is near zero. The sputtered particles are mainly the deposited Ti and adsorbed N.

3. Results and discussion

The agreement between the calculated composition depth profile and the corresponding Auger electron spectroscopy (AES) measurement is shown in Fig. 2 for the sample that was prepared by MIBED on an iron substrate. A transition layer about 20 nm between the film and the substrate is formed according to the simulation calculation, which is of great benefit to the adhesion of the film to the substrate. The transition layer results from the penetration of the incident ions and the collision cascade of the incident ions and target atoms. The N composition profile in the film conforms with the AES result very well, which indicates that the N absorption model is rational.

In order to compare the intermixing effect of Mo ions and N ions, the Mo ions are substituted by N ions in the computer code, so the intermixing layer is formed completely by N ions (Fig. 3). The Ti content in Fe in Fig. 2 is much higher than that in Fig. 3. This indicates that Mo implantation has a stronger mixing effect than

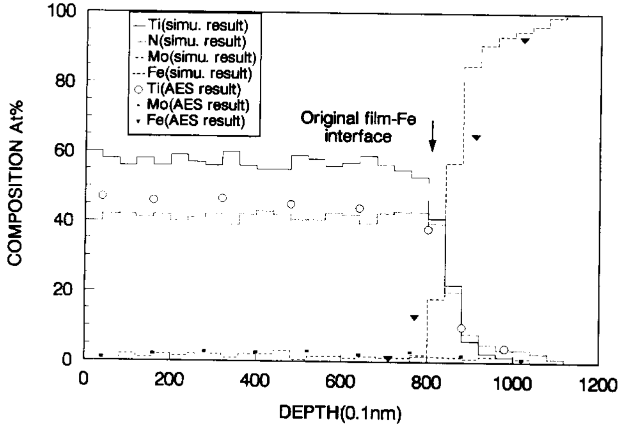

Fig. 2. Simulation result and AES result of composition profile of the (TiMo)N film enhanced by $Mo^+ + N^+$ion beam during deposition. The carbon of AES is ignored. The particle arrival ratio is Ti:N:Mo^+:N^+ = 11:7:1:1.

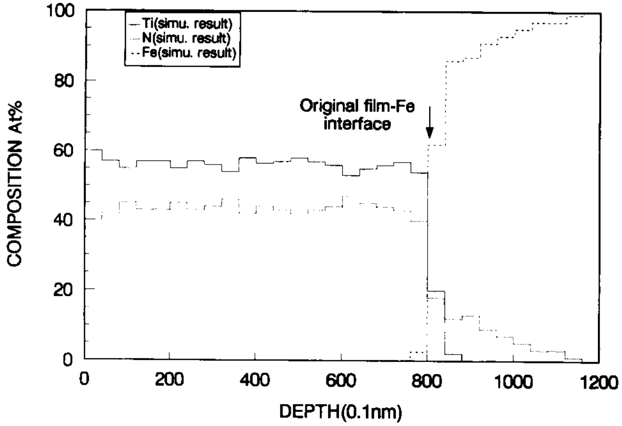

Fig. 3. Simulation result of composition profile of the TiN film enhanced by N^+ ion beam during deposition. The particle arrival ratio is Ti:N:N^+ = 11:7:2.

does N implantation. The strong mixing effect of Mo implantation is because (a) the Mo ion charge state is much higher than that of N, so the Mo ions have much higher energy than do N ions, and (b) the energy transfer T_{Mo} produced by Mo and Ti collisions and T_N produced by N and Ti collisions are:

$$T_{Mo} = 0.89E \sin^2(\theta/2) \quad (4)$$

$$T_N = 0.69E \sin^2(\theta/2) \quad (5)$$

Here E is energy of the incident ion and θ is the scattering angle. The constant 0.89 in Eq. (4) is larger than the constant 0.69 in Eq. (5). All these factors contribute to the strong energy transfer in Mo and Ti collisions and produce a strong mixing effect in the penetration of Mo through the film–substrate interface.

The X-ray diffraction results show that the MIBED film is mainly TiN. For compounds formed from metal and gas elements (O, N etc.) the Bragg rule of electronic stopping has a deviation of 10–40%. The calculated composition profile of Mo conforms to the AES measurement very well in Fig. 2. The film thickness is larger than the range of Mo ions. The Mo profile in the film depends both on the implanted range and on the particle arrival ratio at the film. When the implanted Mo flux is relatively low, the implanted range of Mo has a minor influence on the profile of Mo. In this case, the deviation of the Bragg rule does not make a significant change to the composition profile of Mo.

4. Conclusions

The computer simulation of the (TiMo) N MIBED process can provide many details of the resultant film, such as composition profile and intermixed layer thickness etc. Mo ion implantation has a stronger mixing effect in the film–substrate interface than does N ion implantation. The N profile of the computer simulation conforms to that of the AES results. This indicates that the nitrogen adsorption model used here is rational.

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