

## Composition of Thin C, Ti, Zr and Mo – Based Layers Fabricated on Si by Means of SIAD and Accompanying Radiation Damage of Si Surface

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The development in the structure and composition of C, Ti, Zr and Mo-based layers formed by self ion-assisted deposition (SIAD) of thin films onto silicon when (100)-silicon wafers were floated to a negative potential with respect to the source of 3 kV to accelerate the ion species is reported. Analysis was carried out using RBS/Channeling methods and the RUMP code computer simulation. Elemental analysis of the coatings shows a content of carbon, oxygen, silicon and hydrogen in coatings. A quantitative evaluation of ion irradiation effects during low-energy SIAD of thin films on silicon is given.

### 1. Introduction

There is a much interest for the last decades in the deposition of thin films using ion assistance techniques including direct ion beams [1] or plasma sources [2]. Generally such techniques involve simultaneous bombardment of a thin film during deposition with inert gas ions or chemically active ions to achieve a desired composition. Only in the case of self-ion assisted decomposition [3] can the presence of species, desired or not, different to the deposited species be avoided. Although contamination occlusion in deposited films using SIAD is well known [4] little quantitative information on its concentration or the effects of silicon damage as a function of the processing parameters exist [5-7]. Previously it was reported about the structure and composition of coating/Si constructions fabricated by means of SIAD when the energy of assisting ions was 5, 10 or 20 keV [4, 7, 8]. The present study represents a step in this direction in which, in a resonance vacuum arc source with graphite(C), titanium, zirconium and molibdenium (Me) electrodes is used to produce a mixture of Me(C) and Me<sup>+</sup> (C<sup>+</sup>) ion species for SIAD process when the ion assisting energy was 3 keV.

### 2. Experimental

The system employed for the current study has been described in detail elsewhere [9] and consists, essentially, of a vacuum chamber pumped by diffusion pump to which is attached resonance vacuum arc source. Substrates were (100) silicon wafers and were floated to a negative potential with respect to the source of 3 kV to accelerate the ion species. The number of ions was estimated from integrated current measurements and the neutrals from measurements of film thickness on un-biased substrates over a known period of time. From such measurements it was found that ion/atom (I/A) ratios were between 0.2 and 0.4 and film deposition rates were between 0.3 and 0.4 nm/min. Deposited films were investigated using Rutherford backscattering spectroscopy in conjunction with channeling (RBS/C) of 1.4 MeV He<sup>+</sup> ions. RBS data for concentration against depth were compared with data from the RUMP code simulation [10]. The scattering angle was 168°, the angles of the entry and escape were 0° and 12° correspondingly. The energy resolution of the analyzing system was 17 keV.

### 3. Results and discussion

In Fig.1 the relative concentration of titanium, silicon and accompanying elements carbon, oxygen and hydrogen are plotted vs depth in constructed titanium-base layer/Si structure. The quantitative RBS data in Fig.1 has been obtained from the original spectra using the standard RUMP computer program [10] and predicts that Ti-based film thickness is ~60 nm. This data shows an decrease in Ti concentration of about 50 and more % at the film/substrate interface where the Ti level is less than 1 at %. In addition the RBS data shows the presence of significant level of carbon and oxygen in the film. RUMP simulation of the coating composition indicates that there must also be a significant quantity of hydrogen in the film. This cannot be detected by RBS

directly. But unless significant quantities of H are present in the films the as-measured RBS data cannot be fitted by a RUMP simulation for all of the other measured component peak intensities. Recently conducted experiments using a resonance nuclear reaction  $^1\text{H}(^{15}\text{N},\alpha)^{12}\text{C}$  confirmed the RBS-RUMP data about a huge amount of hydrogen in the coatings prepared by means of SIAD with assisting ions energy between 5 and 10 keV [11].

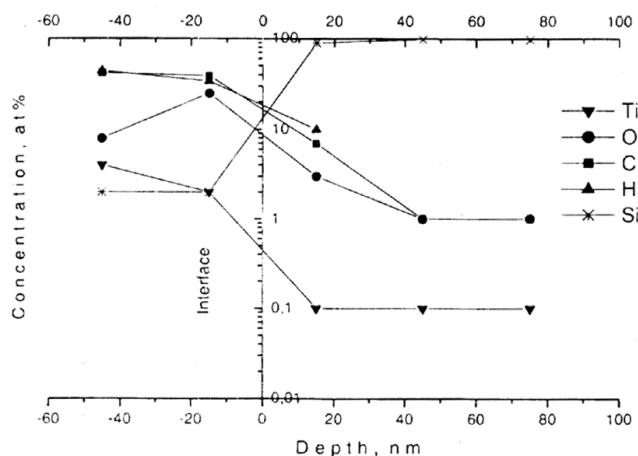


Fig.1. Relative content of species of Ti-based SIAD layer on silicon.

This high C and H content arises because of the used vacuum conditions which allow deposition of hydrocarbons onto the growing film during ion bombardment. Oxygen concentration has a maximum close to the interfacial region. Therefore one may consider an oxide layer on the substrate surface as the main source of O in the fabricated structure. The Ti "tail" in silicon as seen in Fig. 1 indicates that Ti atoms penetrate deep into silicon during SIAD process due to radiation enhanced diffusion stimulated by a high density of energy deposited into collision cascades. The same reason is, probably, a driving force for an out diffusion of Si atoms from substrate into the coating which leads to appearance of approximately 2 at% silicon in the surface film. The qualitatively similar behavior of components of the structures fabricated on Si substrate using deposition of thin films on C, Zr and Mo-base was observed when the energy of the assisting ions was 3 keV.

RBS/Channeling spectra of C and Mo-based thin films deposited and ion-irradiated samples are shown in Fig.2. The level of residual damage in the SIAD treated samples was extracted from the aligned spectra of backscattered ions.

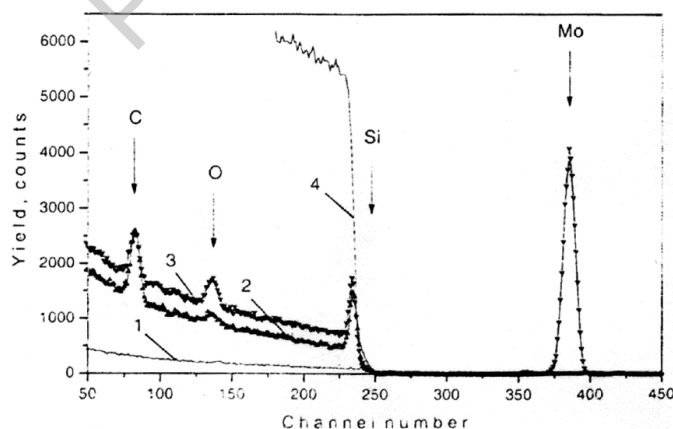


Fig.2. Backscattering/channeling spectra of: 1 – virgin Si, 2 – Si with C-base coating, 3 – Si with Mo-based coating; 4 – random of Si with Mo-based coating.

Since ions that are channeled can only be scattered by atoms that are displaced from the lattice site, the aligned spectra essentially replicated the profile of the interstitially displaced atoms (we neglect a flux peaking effect because of fact that very thin layers are analysed). An increase in the yield in the aligned spectrum corresponds to an increase in the damage or number of displaced atoms. In our experiment we observed that the damage of Si surface increases quite insignificant when Mo<sup>+</sup>-assisting ions are used compare with C<sup>+</sup> ions, curve 2 and 3 in Fig. 2. These results and presented in Table 1 were not expected. Therefore we may suppose that more intense damage annealing takes place in silicon when more heavy ions for ion-irradiation during deposition of coatings are used. Important also is that the level of the damage created in substrate much less then the same observed in [7] where the energies of assisting ions from 7 to 20 keV were used. This fact could be expected, but the most peculiar phenomenon observed here is the increase of the yield of the aligned spectra behind the damage peak under the influence of ion mass (excepting Ti), Table 1, leading to an increase of dechanneling rate as a function of the energy density deposited in collision cascades. This suggests that different types of damage in silicon can be created so that the lattice strain produced by these defects can have influence on the rate of dechanneling. Therefore further structural investigation of SIAD constructed structures should be performed.

Table 1  
System configuration, mass ratio ( $M_i/M_t$ ),  $\chi_{min}$ ,  $Y_{max}/Y_{rand}$  of the coating/Si structures

Base of coating	Si	Mo <sup>96</sup>	Zr <sup>91</sup>	Ti <sup>48</sup>	C <sup>12</sup>
$M_i/M_t$	-	3.43	3.25	1.71	0.43
$\chi_{min}$	3.6	13.4	16.4	7.6	9.4
$Y_{max}/Y_{rand}$	-	0.31	0.32	0.23	0.26

#### 4. Summary

The structure and composition of films formed by deposition C, Ti, Zr and Mo-based thin layers onto silicon using the SIAD have been investigated. Under vacuum condition used (base pressure  $10^{-2}$  Pa), ion to atom ratio 0.2-0.4 and rate of deposition of 0.3-0.9 nm/min the films include not only base-atoms of coatings but also carbon, oxygen, silicon and hydrogen. It is found out that thickness of coating/Si intermixed layer increases with the increase of the ion mass as well as the damage or the amount of displaced atoms in silicon increases. Increasing of the mass of assisting ions leads to the growth of the dechanneling rate in align spectra. The experimental data present the support of the important role of cascade effects in the processes of atomic intermixing and damage creation.

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