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COMPUTER SIMULATION OF TRANSIENT LAYER CHEMICAL COMPOSITION IN Cr-N FILMS OBTAINED BY ION BEAM ASSISTED DEPOSITION

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Проведено комп’ютерне моделювання формування Cr-N плівок, створених за допомогою імплантаційно-стимулюючого осадження (IBAD-метод). Розраховано кількість азоту у зростаючій плівці хрому, а також рівень створюємих іонами азоту дефектів. Проаналізовано співвідношення між розподіленням дефектів та кількістю хрому в залежності від товщини плівки.

Проведено компъютерное моделирование формирования Cr-N пленок, полученных с помощью имплантационно-стимулированного осаждения (IBAD-метод). Рассчитано содержание азота в растущей пленке хрома, а также уровень создаваемых ионами азота дефектов. Проанализировано соотношение между распределением дефектов и содержанием хрома в зависимости от толщины пленок.

The computer simulation of Cr-N film deposition by IBAD method was carried out. The implanted nitrogen content in the growing film is calculated, values of the radiation defect formation in the film are obtained. The variation of the implanted nitrogen relationship to the defect distribution in the growing film depth is analyzed.

Now the ion- and ion-plasma technologies are widely used to the material surface layers hardening. Ion-beam assisted deposition (IBAD) is one of the method to produce the protective coatings. This method consists in the film deposition from vapour phase with the simultaneous bombardment by the energetic ions. Chemical active elements are used as ions; it allows to produce the films with different chemical and phase composition.

The high adhesion of films with the substrate is one of the problem. This problem can be solved by the transient (or so called adjoined) layers formation. These layers have the smooth changeable characteristics on distances lower than the film thickness. On IBAD use one can obtain the transient layers with controlled thickness and the chemical composition instead of the sharp boundary between the deposited film and the substrate.To predict the obtained coatings properties it is necessary to calculate the implanted ions concentrations also as the produced radiation defects in these layers.On the irradiated film growth the thermal vapoured atoms deposit on the surface, the implanted atoms introduction occurs with the atomic damage cascades and the ion stirring ;the surface atoms sputter. The radiation defects diffusion and the implanted impurities diffusion is observed to the surface and to body sinks. As a result of diffusion processes the phase precipitation and the nanostructure production are observed.

Let us consider only the primary processes of the impurity implantation and of the radiation defects formation. It is known [1] that on the sputtering the atoms of near surface layers are knocked out. At the ion energy of several keV the impurityis implanted in the bulk of material, the sputtering rate is entirely defined by deposited from vapour phase atom layer and didn`t depend on the implanted ion dose. So , the film growth rate doesn`t depend on the implanted ions dose. According to this we can represent the film growth in the following way. In the steady-state condition the film boundary moves uniformly with rate **v** along the axis **x**. The implanted ion profile **f(x)** shifts with the growing film boundary. In time **t** at the point **x** the implanted atoms concentration will vary by quantity $D(x) = N\int f(x,t)dt$, where N- bombarding ions density.

In general the interstitial impurity profile is a function of implanted atoms dose. With the low concentration this dependence can be neglected. As we consider the steady state process of the film growth with the constant rate $f(x,t) = f(x-vt,0)$. Then $D(x) = N$. Thus to obtain the impurity concentration in the growing film it is necessary to know the implanted ion deposition profile.

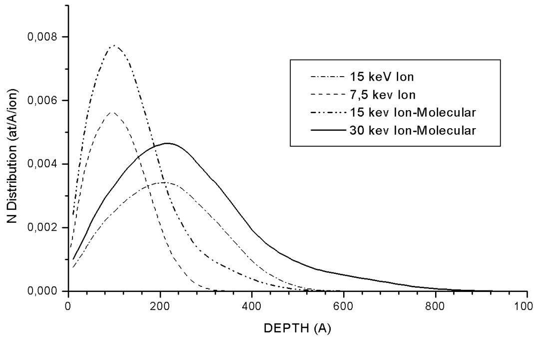


Fig.1. Implanted nitrogen distribution in depth of Cr on N implantation of atomic beams with energies of 7,5 keV, 15 keV and ion-molecular beams with energies of 15 and 30 keV, containing 40% and 50 % of molecular

nitrogen

To the calculation of implanted ion deposition profile so as to damage profile calculation the program of computer simulation of atom-atom collision cascades by method Monte-Carlo SPURT [2] was used. According to the program SPURT the atom-ion interaction is simulated by twin collision method [3]. The main assumption of twin collision approximation consists in that the moving atom in a time interacts only with one target atom. The ion interaction is the elastic one. On moving between the collisions the particle loses energy in the electron subsystem interaction. The non local model of the electron losses was used in the program .The process of atom-ion flux interaction with the solid surface was simulated as the stochastic process consisting of the isolated ions incidence .The processes of cascade overlap were neglected.

The computation was carried out for the deposited films of Cr bombarded by nitrogen ions. The ion beam variables corresponded to the NSC KIPT assembly “Argo-1” [4]. The molecular-atomic beam with 40% of atomic and with 60 % of molecular nitrogen was used. The beam energy ranges in 15…30 keV. As the binding energy of nitrogen atoms in the molecule is considerably lower the beam energy the molecular beam with density N and the energy E was considered in the computation as the particle beam with energy E/2 and with density 2N. It was assumed that after the molecule break-down atoms on the surface dosn’t effect on the evolution of atom-atom cascades in the bulk material. In Fig.1 the results of deposit profiles of nitrogen atoms from the ion beams of energy 15 and 7,5 keV and from ion-molecular beams of energy 15 and 30 keV are presented. The deposition profile of atomic-molecular beams was obtained by the superposition of ion beams with energies of E and 0,5E with weight 0,4 and 0,6 correspondingly.

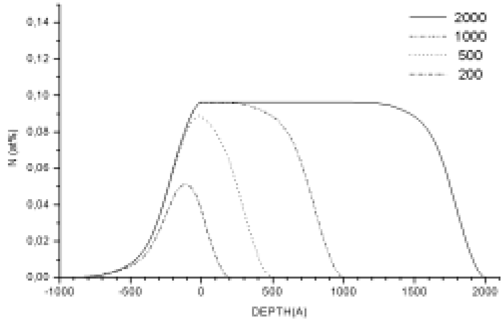


Fig.2 Distribution of nitrogen in depth of growing Cr film in atomic percents under N implantation of atomic-molecular beam with energy 30 keV containing 40% of monatomic and 60 % of molecular nitrogen. The ion flux-10^{14}(cm^2sec^{-1});the film growth rate-2Å/sec. The different curves correspond to the different thickness of the deposited film. The deposited film thickness is given in Å.

As it is seen from figure nitrogen atoms of ion-molecular beam with energy of 15 keV penetrate into the target on depth up to 600 A and with energy of 30 keV-on depth up to 1000 A. The implanted atoms deposition depth causes the characteristic thickness of transient interfaced layers between the bulk material and the deposited film. Nitrogen deposition profiles obtained by this method allow to calculate nitrogen distribution in the growing film of Cr. On Fig.2 and on Fig. 3 the calculated nitrogen concentration on it’s implantation from ion-molecular beam of energies of 30 and 15 keV with beam characteristics of assembly “ARGO-1” are presented. The depth values lower 0 correspond to the bulk material. It is seen in figures that the transient layer thickness increases with the energy increase. At energy of 30 keV the interfaced layer extent runs into 800 A. When the deposited film thickness increases the nitrogen content attains the constancy and for the thickness higher of 1000 A nitrogen implanted content is invariable. The impurity content decreases sharply on approach to the surface. At energy of 30 keV the transient layer thickness is lower 500 A and at energy of 15 keV it is lower 300 A.

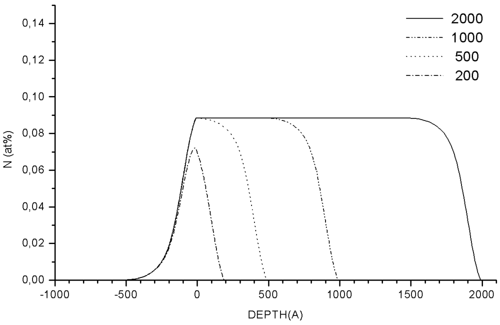


Fig.3. Distribution of nitrogen in depth of growing Cr film in atomic percents under implantation of atomic-molecular beam with energy 15 keV containing 40% of monatomic and 60 % of molecular nitrogen. The ion flux-10^{14}(cm^2sec^{-1});the film growth rate-2Å/sec. The different curves correspond to the different thickness of the deposited film. The deposited film thickness is given in Å

Fig.4 represents Cr-N equilibrium diagram. As one can see on diagram, nitrogen ions introduced in the specimen may form some chemical composition with Cr. Fig. 3 and Fig. 4 demonstrate that nitrogen content corresponds to the mixture of Cr and Cr N at the used rates of the coatings deposition and at the given beam characteristics. Varying the beams parameters or the deposition rate one can change considerably the impurity content in the transient layers.

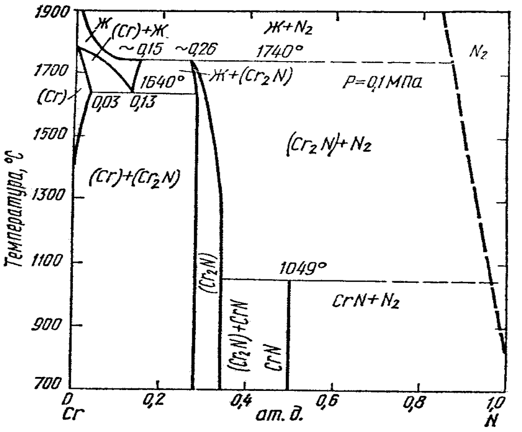


Fig.4.Equilibrium phase diagram Cr-N.

The presented equilibrium diagram may vary under irradiation due to the introduction of large number of radiation defects (vacancies and the interstitial atoms). The inhomogeneous non-equilibrium defect concentration in the film depth may change considerably the kinetics of structure formation in different layers of the film. Therefore let us consider the growing film radiation damage in depth. On Fig. 5 the profile of defect formation in Cr under nitrogen ion bombardment together with the introduced nitrogen profile are presented.

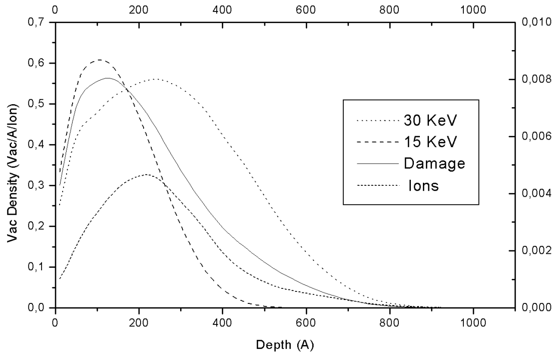
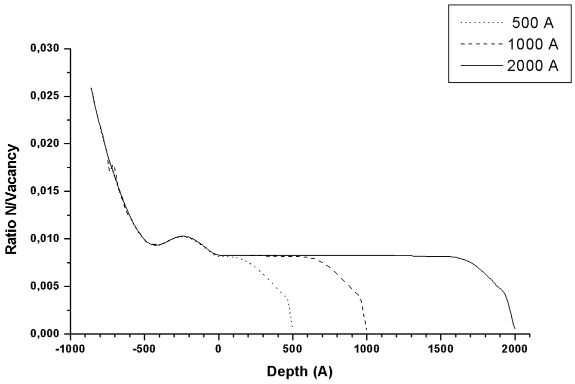


Fig. 5. Radiation defects distribution in Cr depth under N implantation of ion beams with energies 15 and 30 keV and ion-molecular beam with energy 30 KeV containing 40% of monatomic and 60 % of molecular nitrogen. The implanted nitrogen profile is presented for comparison. The upper and the right axis represent the implanted ion profiles

It is seen that at the given beam energy the formed Frenkel pair number 100 times as large as the introduced impurities content. It demonstrates the considerable effect of the radiation defects in the film structure formation. To obtain the resistant coating it is necessary to provide the uniformity of the ratio impurity/defect(η) in the film depth. On Fig. 6 the results of such computations for different film thickness are presented.



As it is seen on Fig. 6 the equilibrium ratio η is attained along the film. In the near surface regions the coefficient η decrease is observed. It is due to the fact that the radiation defects formation is more intensive near surface; the impurity deposition maximum is displaced to the material depth. For the film thickness higher than 1000A the value η is constant in the film depth that proves the film uniform composition at such thickness.

Fig.6. The ratio of nitrogen implanted atom content in depth of Cr growing film on N implantation of beam with energy 30 keV and containing 40 % of monatomic and 60 % of molecular nitrogen. The different curves correspond to the deposited film different touchiness. The film thickness is given in Å

In the presented paper the computer simulation of Cr-N film deposition by IBAD method was carried out. The implanted nitrogen content in the growing film is calculated, values of the radiation defect formation in the film are obtained. The variation of the implanted nitrogen relationship to the defect distribution in the growing film depth is analyzed; the way of the film interfaced layer chemical and phase composition variation is proposed.

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