

## Informatics support of thin film deposition with specified structure development

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**Abstract.** Virtual experiment method which consists of acquisition, systematization, and analysis of large experimental results of thin film deposition technology is described. The data base examples and thin film deposition of any materials result analysis are adduced. Dependence of thin films structure from thin film deposition rate and method and substrate temperature is shown. DLC thin films with amorphous and crystalline structures deposition regimes are represented. WSi thin films for using as thin film resistor in microcircuit and as a superconductor coating in one photon detectors are described. It is shown that the elaborated method of informatics support of research and development in the field of thin film deposition technology gives opportunity to analysis and choose of thin film deposition method and regimes for manufacturing of thin films with specified structure and characteristics.

“Doing anything well, take some information” – thus sounds the motto of a number of successful researchers and businessmen and others. So the item of this article – the reasoning of relevance and practicability of creation of a methodic providing of a research in the field of thin film deposition with some information is actual task. This methodic is intended for science beginners studying, and for specialist for deciding new tasks, as well.

The suggesting methodic consists of acquisition, systematization, and analysis of large number of publications and experimental results of thin film deposition technology by means of a special algorithm, and it's representing as the relation data base [1].

The results of information analysis, which may be carried out by means of the data base control systems, one can represent in a view of curves and histograms and other methods of information representation. These are a virtual experiment results, in substance.

As an example, the information about materials, deposition methods and regimes of thin film technology is shown in table 1. The parameters of the data base were chosen on the base of work experience with data base control systems and on the reasoning of relevance to research of thin film deposition method and regimes influence to thin films structure.

So, the results of publication analysis for thin film deposition of silica, aluminum oxide, ITO, titanium nitride, bismuth telluride, and DLC are represented in the table 1. Atomic Layer Deposition (ALD) and Chemical Vapor Deposition (CVD) and Plasma Enhance Chemical Vapor Deposition (PECVD) and Electron Beam Evaporation (EBE) and Pulsed Laser Deposition (PLD) and Magnetron Sputtering (MS) and Arc Evaporation (Arc) and Ion Beam Deposition (IBD) methods are represented in the table 1, as well. There are analyzing some parameters of thin film deposition such as particle energy (E), deposition rate ( $V_d$ ), substrate temperature ( $T_s$ ), gas pressure into vacuum chamber (p), thin film structure in the table 1.



To deposit of thin film with crystalline structure we have to know thin film structure influence from thin film deposition regimes. Well known models of thin films grow do not give opportunity to have common dependence of thin film structure from thin film deposition regimes. It is necessary to have thin film structure dependence from variated process parameters. Thin film deposition rate, atoms and molecules energy, substrate temperature, gas pressure into vacuum chamber are such parameters.

**Table 1.** Thin film deposition methods and regimes data base example.

Thin film material	Method	E, eV	$V_d$ , nm/s	$T_s$ , K	p, Pa	Thin film structure
Al <sub>2</sub> O <sub>3</sub>	ALD	0,05	0,01	873	100	Crystalline
Si	CVD	0,06	10	1075	150	Crystalline
Bi <sub>2</sub> Te <sub>3</sub>	PLD	400	0,4	523	10 <sup>-3</sup>	Crystalline
InSnO (ITO)	EBE	0,2	0,24	373	2·10 <sup>-2</sup>	Amorphous
AlN	MS	4	0,1	573	10 <sup>-2</sup>	Crystalline
ZnO	PLD	1000	0,01	573	10 <sup>-5</sup>	Crystalline
DLC	PE CVD	10	1	350	2	Amorphous with crystals
DLC	PE CVD	300	80	1200	2	Crystalline
DLC	Arc	10	8	293	10 <sup>-3</sup>	Amorphous
DLC	Arc	10	100	373	4·10 <sup>-6</sup>	Amorphous with crystals
DLC	IBD	70	0,02	473	10 <sup>-2</sup>	Amorphous with crystals
DLC	IBD	100	0,05	900	10 <sup>-2</sup>	Monocrystalline
DLC	EBE	0,2	0,8	293	10 <sup>-3</sup>	Amorphous
DLC	EBE	0,2	5	573	10 <sup>-3</sup>	Crystalline
DLC	PLD	0,5	0,1	453	10 <sup>-4</sup>	Amorphous with crystals
DLC	PLD	400	10	773	10 <sup>-4</sup>	Monocrystalline

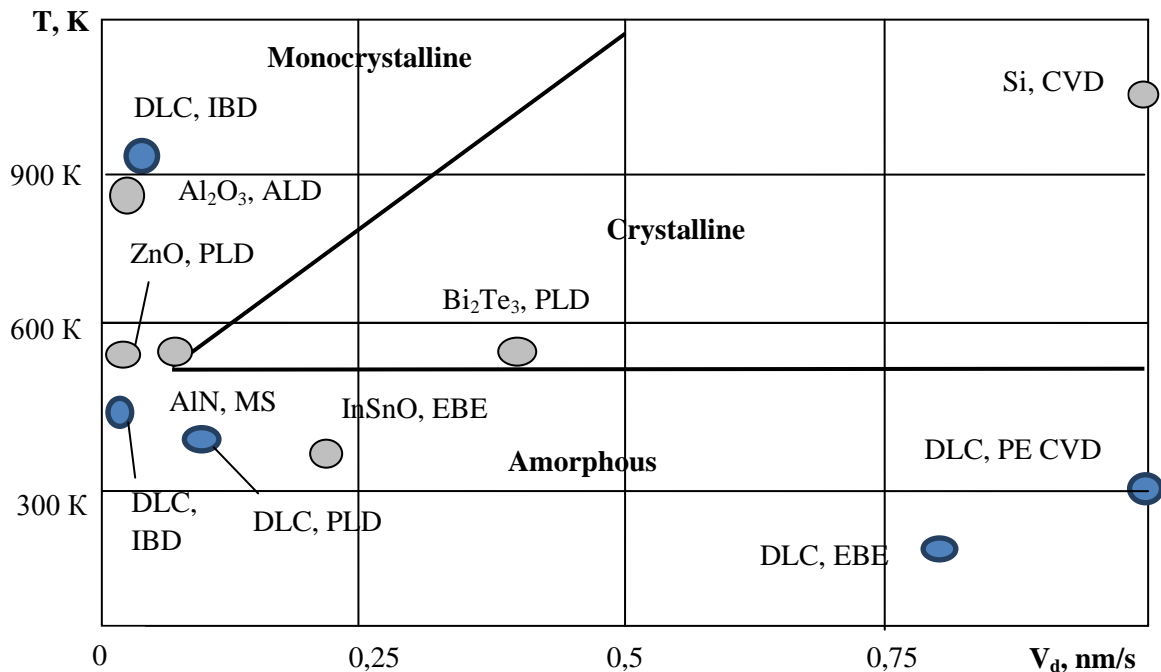
For ease of representation of thin film deposition regimes influence to thin film structure it is marked, in two dimension coordinate system “thin film deposition rate – substrate temperature”, the areas of thin film deposition methods and thin film materials and structures from literature and data base in table 1 (figure 1). Lines of Ge thin film structure junction from amorphous to crystalline and monocrystalline condition are marked by solid lines in figure 1 [2]. We have an opportunity to compare and analyze of results of new research by means of this plot – so we have opportunity to carry out of virtual experiments.

As it follow from figure 1, the results of virtual experiments with thin films from different materials and deposited with different regimes are coincided with the results of Ge thin film deposition real experiments as a rule (solid lines in figure 1).

More detailed analysis of literature [3–6] and other tables of elaborated data bases give opportunity to resume the next:

- Thin films with amorphous structure can be manufactured without substrate heating even and with any thin film deposition rate. So, we may resume that all thin films deposited with room temperature of substrate have amorphous structure. But thin film epitaxy can be happened with room temperature of substrate and with very small thin film deposition rate.
- Thin films with crystalline structure can be deposited to any substrate materials with melting temperature more than 600–700 K by means of any thin film deposition method and with any thin film deposition rate.

- Besides this, thin films with crystalline structure can be manufactured by means of substrate heating to 600 K and more. In addition, thin film deposition rate must be more than 0,2–0,25 nm/s, and there are not limit of thin film deposition rate maximum.
- Thin films with mono crystalline structure can be manufactured with very small thin film deposition rate (less than 0,2–0,25 nm/s) and with high substrate temperature (more than 600 K).
- Besides this, thin films with mono crystalline structure and with diminution minimum can be manufactured by means of ion beam deposition method with particle energy  $E=4$  keV, substrate temperature  $T_s=800$  K, thin film deposition rate  $V_d=0,5$  nm/s and ionization degree  $k=0,1$  %.

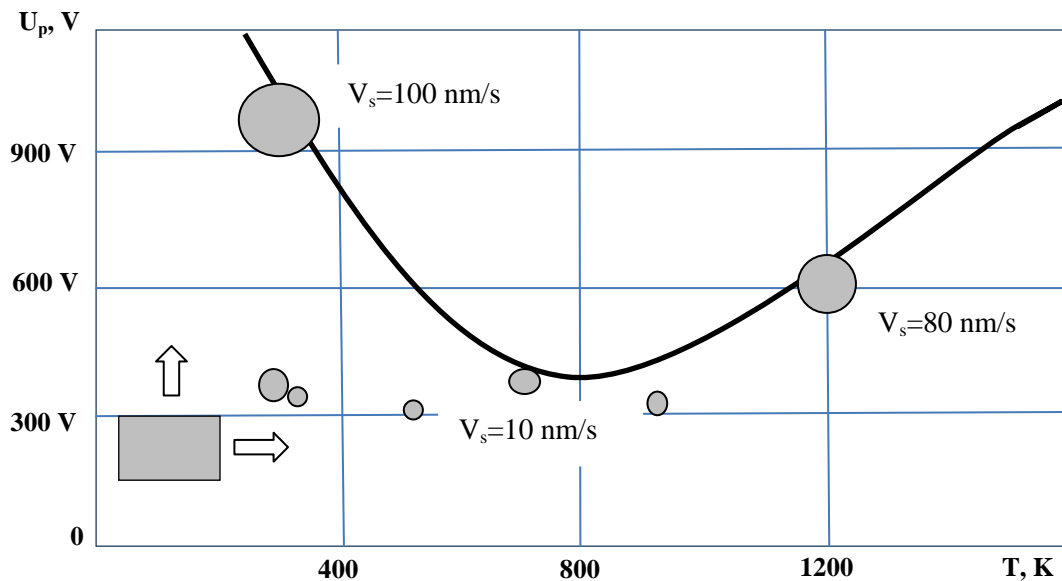


**Figure 1.** Dependence of thin films structure from thin film deposition rate  $V_d$  and method and substrate temperature  $T$ .

The experimental research results of DLC thin film deposition with plasma discharge voltage  $U_p$  and substrate temperature  $T$  are represented in figure 2 (the rate of DLC thin film deposition is corresponded with the circle diameter). This results were provided with the help of dates in table 1. In the left down corner of figure 2, regimes of DLC thin film deposition on laboratory coater is shown and some variants of DLC thin film deposition rate increase by means of plasma discharge voltage  $U_p$  or substrate temperature  $T$  increasing are represented.

It is impossible to obtain the same results by means of real experiments because the real experimental equipment has, as a rule, only one or two source of thin film deposition and it has not opportunity to diversify in a large range of thin film deposition regimes such as particle's stream intensity and energy, gas pressure into vacuum chamber, substrate temperature and so on.

WSi thin films are used as a thin film resistor in microcircuit and as a superconductor coating in one photon detectors [7–10]. Thickness of WSi superconductor coating must be less than 10 nm, and the main methods of WSi thin film deposition are PLD and ion plasma sputtering and CVD, as well. Thin film deposition rate is depended from thin film deposition method and has amount variation from 0,032 to 2,5 nm/s (table 2). Thin film deposition method with productivity maximum is CVD method, whereas PVD thin film deposition method has limit about 0,7 nm/s. Thin film deposition method with particle energy maximum (10–1000 eV) is PLD method. WSi thin films can be manufactured by means of ion plasma sputtering of multicomponent WSi target or of two targets made of W and Si.



**Figure 2.** The influence of DLC thin film deposition rate maximum from substrate temperature  $T$  and plasma discharge voltage  $U_p$  (rectangle in the left corner is the working regimes of the laboratory coater).

**Table 2.** WSi thin film deposition rate and particle energy with some thin film deposition methods.

Thin film deposition method	Thin film deposition rate, nm/s	Particle energy, eV
PLD	0,032 – 0,7	10 – 1000
Ion plasma sputtering	0,39 – 0,71	1 – 10
CVD	1,33 – 2,5	0,05 – 0,1

Comparison of any materials thin film deposition regimes shown that thin film nanostructured condition is realized in a restricted diapasons of particle mass and energy streams.

So, the elaborated method of informatics support of research and development in the field of thin film deposition technology gives opportunity to analysis and choose of thin film deposition method and regimes for manufacturing of thin films with specified structure and characteristics.

The virtual experiment method is recommended for using in the automatic expert systems for decide of development modern equipment begin, of resource assignment to buy of available equipment or to correct of thin film deposition regimes of operated equipment for manufacturing of thin films with specified structure. By means of automatic expert systems one can evaluate the prospect of a process and equipment stock or newly creating and analysis of modern process and equipment progress. Predict of thin film with specified structure deposition opportunity, and carry out of design expertise, practicability of a very expensive equipment procurement, and of research and development and engineering operations financial support request expertise, as well.

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