6.1. Thin Film Science

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6.1.1. Introduction

In recent years, thin film science has grown world-wide into a major research area. The importance of coatings and the synthesis of new materials for industry have resulted in a tremendous increase of innovative thin film processing technologies. Currently, this development goes hand-in-hand with the explosion of scientific and technological breakthroughs in microelectronics, optics and nanotechnology [1]. A second major field comprises process technologies for films with thicknesses ranging from one to several microns. These films are essential for a multitude of production areas, such as thermal barrier coatings and wear protections, enhancing service life of tools and to protect materials against thermal and atmospheric influences [2, 3]. Presently, rapidly changing needs for thin film materials and devices are creating new opportunities for the development of new processes, materials and technologies (Fig. 6.1).

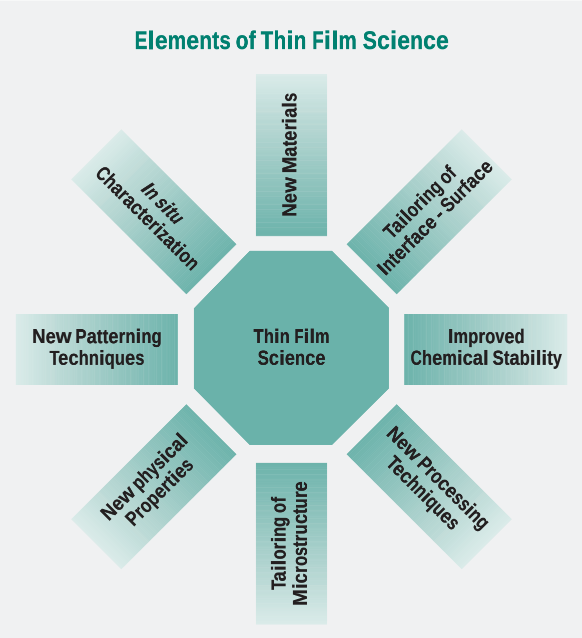


Fig. 6.1. New processing techniques related to thin film materials and devices.

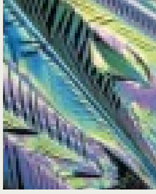
Therefore, basic research activities will be necessary in the future, to increase knowledge, understanding, and to develop predictive capabilities for relating fundamental physical and chemical properties to the microstructure and performance of thin films in various applications. In basic research, special model systems are needed for quantitative investigations of the relevant and fundamental processes in thin film materials science. In particular, these model systems enable the investigation of i.e. nucleation and growth processes, solid state reactions, the thermal and mechanical stability of thin film systems and phase boundaries. Results of combined experimental and theoretical investigations are a prerequisite for the development of new thin film systems and the tailoring of their microstructure and performance.

6.1.2. State of the Art

The major exploitation of thin film science is still in the field of microelectronics. However, there are growing applications in other areas like thin films for optical and magnetic devices, electrochemistry, protective and decorative coatings and catalysis. Most features of these thin film activities are represented by a relatively new research area, called *surface engineering* [2]. *Surface engineering* has been one of the most expanding scientific areas in the last 10 years and includes the design and processing of surface layers and coatings, internal interfaces and their characterization. Surface engineering is directed by the demands of thin film and surface characteristics of materials.

(a) Thin film processing techniques

There exists a huge variety of thin film deposition processes and technologies which originate from purely physical or purely chemical processes. The more important thin film processes are based on liquid phase chemical techniques, gas phase chemical processes, glow discharge processes and evaporation methods [4]. Recently, a considerable number of novel processes that utilize a combination of different processes have been developed. This combination allows a more defined control and tailoring of the microstructure and properties of thin films. Typical processes are e.g. ion beam assisted deposition (IBAD) and plasma enhanced CVD (PECVD). Examples for novel thin film processing techniques, which are still under development, are pulsed laser ablation (PLD) and chemical solution deposition (CSD). Both techniques enable the synthesis of complex thin film materials (complex oxides, carbides, and nitrides).



Presently, experimental efforts are increasingly supported by computational approaches that address complex growth processes, saving time and money. These approaches enable e.g. the description of the evolution of thin film microstructures as a function of processing parameters.

(b) *In situ* characterization

The thin film process equipment can be categorized into production equipment for device manufacturing, equipment for research and development, and prototype apparatus for fundamental investigations of new or established deposition processes. One reason for the world-wide rapid growth of deposition technology is that equipment manufacturers have successfully met the demands for more sophisticated deposition systems including *in situ* characterization (e.g. reflection high-energy electron diffraction (RHEED), scanning probe microscopy (SPM)) and process monitoring techniques for measuring process parameters and film properties (e. g. ellipsometry, plasma analysis techniques). Novel experimental tools have enabled discoveries of a variety of new phenomena at the nanoscale which have in turn opened unexpected opportunities for the development of thin film systems, and tremendous progress regarding a fundamental understanding of the respective technological processes has been made.

(c) New materials

Thin film systems necessitate direct control of materials on the molecular and atomic scale, including surface modifications, deposition and structuring. Many of these techniques were improved during the last decade, resulting in remarkable advances in the fundamental understanding of the physics and chemistry of thin films, their microstructural evolution and their properties. This progress has led to the development of new materials, expanded applications and new designs of devices and functional thin film systems. One of the most outstanding examples is the successful development of semiconductor devices with novel materials like oxides and nitrides (e.g. GaN). Other typical examples are advances in the synthesis of hard coatings based on borides, carbides and nitrides [3].

and the thermal and environmental stability of thin film systems. Future developments are critical to overcoming obstacles to miniaturization as feature sizes in devices reach the nanoscale. Basic research in this field will refer to developments of experimental tools necessary to *in situ* characterize and measure thin film structures (e.g. optical and magnetic characterization), and developments of novel techniques for synthesis and design. These techniques may be more reliable, less expensive, or capable of producing films with new or improved properties. Typical examples are chemical solution deposition (CSD), including hydrothermal approaches, biomimetic pathways for assembling inorganic thin films, or device applications of liquid crystalline polymer films [5].

Experiments alone will be insufficient. Theory and modelling are essential for a complete understanding of the fundamental growth and deposition processes. Multiscale modelling of thin film and nanostructuring processes will be an absolute necessity in the next decade in order to utilize the tremendous potential of thin film science and technology. It is expected that time consuming and expensive experiments will be replaced by theory and modelling.

Especially, it is still necessary to develop a fundamental understanding of the decisive growth and deposition processes. It will be important for research institutes to focus on the development of fundamental and novel processes and devices. This will only be realized if a more defined connection of the activities between single research groups and industry can be achieved, based on a fluent exchange of information. Research institutes and companies, which cannot achieve this, will have difficulty competing in future. In this field, Europe must compete directly with the U.S. and Japan. In comparison to Europe, there appears to exist an advantageous research environment in the U.S. and Japan, which supports a more fluent conversion of results from basic research into applications. This could be balanced in Europe by improved networking between industry and research laboratories in the field of basic research.

6.1.3. Expectations 2000 – 2010

The gap between solving fundamental materials problems and developing new thin film devices for microelectronic and nanotechnological applications is quickly increasing. For example, in many applications the development of thin film systems is accompanied by a variety of materials and processing problems, which require extensive future efforts to be solved. Prominent examples are the adhesion

6.1.4. Expected Needs 2000 – 2010

(a) Initiatives

Emphasis should be placed on future developments of film deposition processes for application in advanced microelectronic device and nanotechnology applications that require the most demanding approaches. Surface engineering is a second important field where similar demands have to be fulfilled. Effective development of thin film systems can only be realized if the fundamental process steps are well understood. For the future advancement of thin film research and technology, the following endeavors are prerequisite:

- Development of improved and novel thin film process technologies and design methodologies
- Development of new materials
- More fundamental understanding of the relationships between microstructure and properties, and how these can be tailored
- Improvement and automation of *in situ* characterization tools with high spatial resolution and chemical sensitivity
- Strong networking between research laboratories and industry in Europe, and materials research centres in Europe, U.S. and Japan
- Establishment of special competence centres

In the following, some examples are given where new processes and technologies will challenge established procedures:

(b) Thin film model systems

Deposition processes for applications in advanced *microelectronics* and *surface engineering processes* will require the most demanding approaches in the near future. New concepts and design methodologies are needed to create and synthesize new thin film devices and to integrate them into architectures for various operations. Examples are the control of surface processes, the development of computer memory chips, and the production of two- and three-dimensional nanostructures. There will be a rapid increase in the significance of *basic research* projects due to the need of new materials and devices in these fields. Therefore, purposeful future developments and an understanding of the versatility of the basic deposition processes is needed, including microstructural evolution of thin films, e.g. substrate and surface preparation, nucleation and growth. For the realization of thin film systems, it is of future interest to understand the critical role of surfaces and interfaces. We need to know the structure and bonding at heterophase interfaces and grain boundaries, and we have to understand how to produce special interfaces experimentally and how to tailor them for specific properties. Additionally, the thermal, chemical and structural stability of the thin film systems and devices need to be investigated thoroughly to allow for the adaptation of fundamental processes. To initiate all these processes, special model systems have to be synthesized and studied experimentally and theoretically (Fig. 6.2).

Typical examples are:

- metal and ceramic multilayers
- functionally graded thin films
- growth of metastable phase layers
- super hard thin films
- nanocrystalline layers
- superlattice thin films
- composite coatings

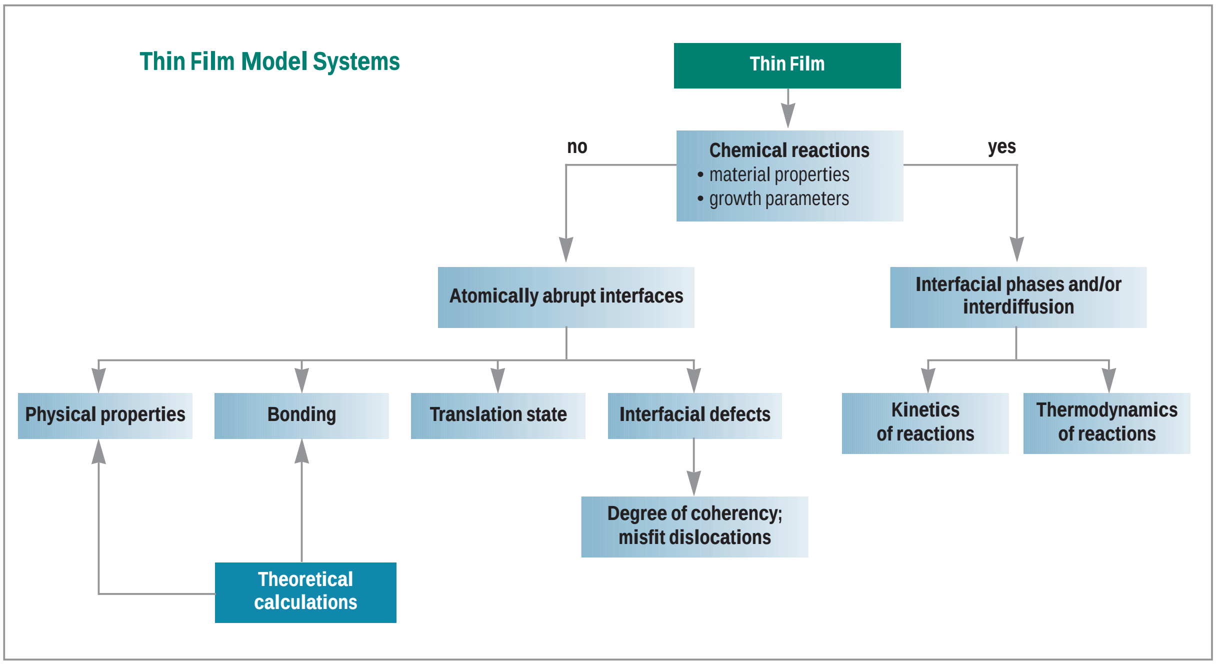


Fig. 6.2. Research areas for thin film systems.

Significant improvement in both, theory and modelling are necessary to help direct the developments in thin film science and technology. This is one of the most promising attempts for accelerating future developments.

(c) The development of new materials: a combinatorial approach

An accommodation of the equipment to the research and development of new device structures and materials with new properties must be performed continuously. For example, research and development equipment has to offer a high degree of flexibility in the accommodation of a multitude of substrates, in deposition parameters, and in real time monitoring capability. Until recently, these facilities did not facilitate a high product throughput, which made the development of new thin film materials rather tedious. By using a *combinatorial approach*, parallel thin film processing can be realized, and by significantly reducing sample size, time and money can be saved (Fig. 6.3).

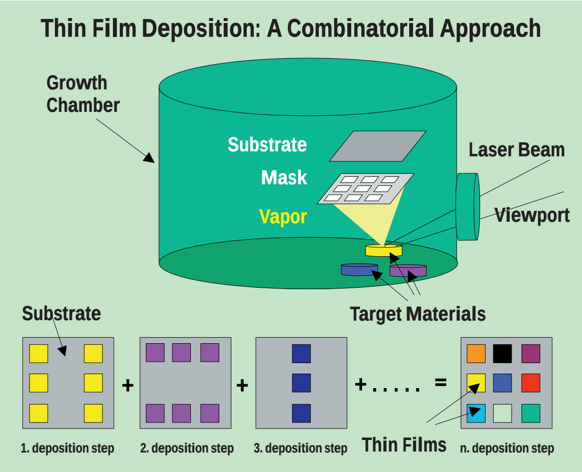


Fig. 6.3. A combinatorial approach for parallel thin film processing.

This requires the development of new and complex deposition systems. For example, this can be realized by using masks with different patterns in front of the substrate. Then, single or/and multi-beam deposition will result in parallel thin film processing. As a result, the substrate will consist of thin film patches with varying chemical composition. However, miniaturization complicates the processing procedures, and thus an improvement in the resolution of typical thin film characterization tools will be of great importance. Full automation of the deposition and characterization routines is required here (e.g. automatic shutter and temperature control, scanning beam RHEED systems). A further advantage of the combinatorial approach is the fast characterization of the deposition process and the system itself. Worldwide, the developments of these processes are still in the initial stages. Presently in Europe, projects of combinatorial chemistry are supported in the field of chemical technologies. These research programmes should be extended to all fields of new technologies, which depend on thin film science, and technology, and it is important to realize these projects in Europe through networks which consist of research centres and industry.

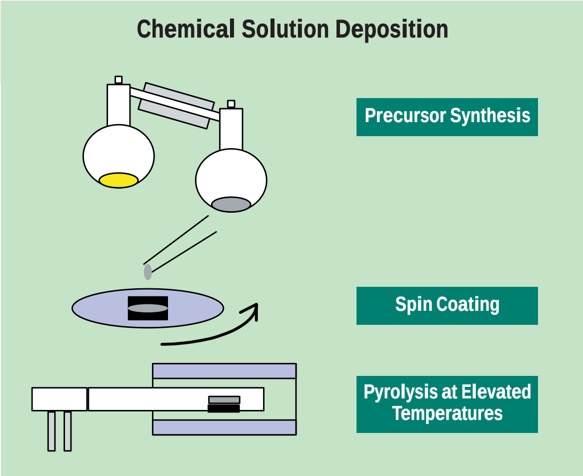


Fig. 6.4. The chemical solution deposition method for the production of epitaxial inorganic thin films.

(d) Thin film systems via chemical solution deposition (CSD)

Conventional CVD and PVD processes are used routinely to synthesize thin film systems. Such process technologies are rather complex and expensive [4]. Depending on the applications, these films have to fulfil special demands and very often, low defect densities are necessary. For most applications, one would prefer films with which have a special texture, low grain boundary density, and smooth surfaces. Epitaxial films fulfil these requirements. Very promising approaches to synthesis inorganic single crystalline thin films are chemical solution deposition method (CSD) (Fig. 6.4) and related processes.

CSD enables the growth of thin films fom solutions, either aqueous or organic [6]. These solutions contain precursor molecules for a variety of elements in the thin film of interest. CSD is inexpensive and enables the synthesis of thin film materials with complex chemical compositions. The main advantage of CSD is the high degree of compositional control, inherent with other solution synthesis routes for multi-element, inorganic materials. Recently, single crystalline carbide and nitride thin films were synthesized via CSD. CSD will become one of the key technologies to synthesize epitaxial oxide, nitride and carbide films for a variety of different applications, e.g. opto-electronic device applications, hard coatings and dielectric thin films. A further advantage of CSD will be the possibility of direct patterning of thin films via stamping techniques. However, for these purposes, appropriate precursor solutions have to be synthesized in future. One big challenge is the synthesis of precursor materials with well-defined doping levels for thin film applications in electronic devices.

(e) Manpower, interdisciplinary research

Continued progress in thin film research seems to be increasingly dependent upon collaborative efforts among several different disciplines, as well as closer coordination among funding agencies and effective partnerships including research laboratories, universities, and industry. Recently, a variety of different interdisciplinary programmes for nanotechnology and microelectronics were initiated in the U.S., Japan and Europe. However, the topic of thin film science and technology is automatically included in such programmes, although it would be of great benefit to establish individual programmes, which focus on major thin film activities in Europe. Interdisciplinary programmes of *combinatorial materials science and technology of thin films* and *surface engineering* are necessary, to promote the formation of fundamental associations for the improvement and development of new techniques, and of novel materials and their properties.

The university education of researchers working in the thin film area would benefit from an interdisciplinary approach. The materials problems in thin films research are very complex and require interdisciplinary training, that is, a combination of studies including physics, chemistry, engineering, materials science and biology. In comparison to Europe and Japan, the U.S. seems to occupy a leading position in this field. In the future, efforts should be taken to compensate for this deficit in Europe by modifying the education system in such a way that new training directions are included, helping to create a new generation of researchers who work across traditional disciplines. This task may be supported by new centres of excellence in the field of thin film science and technology.

6.1.5. Expenditures

Thin film process techniques and research are strongly related to the basic research activities in nanotechnology. Thus, government expenditures on nanotechnology research are a reliable indicator of the budget for thin film research. The government expenditures for nanotechnology research are presently at similar levels in the U.S., Japan and Western Europe, suggesting that the respective quantities of research activity are comparable. According to a WTEC study in 1997 [1], large companies in Japan and the U.S. contribute to research to a greater extend than do their counterparts in Europe. While large multinational companies are developing nanotechnology research activities worldwide, the transfer of new processes to the market is strongest in the U.S. In Western Europe, a diverse combination of university research, networks and national laboratories with a special emphasis on coatings is active. The largest funding opportunities for nanotechnology are provided by the NSF in the U.S., by MITI in Japan and by BMBF in Germany. Categories such as physical and chemical technologies, materials research, microsystem technologies, electronics and nanotechnologies are supported by BMBF. Common features of these disciplines are projects which are located in the area of thin film research. In the case of nanotechnology, the BMBF has established several centres of competence with emphasis on such topics as opto-electronics, nano-analytics, and ultra-thin films. Ultra-thin films are among the main elements of thin film science that have varied applications in optics, microelectronics and wear protection.

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