

MOLECULAR BEAM EPITAXY

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Abstract. Molecular Beam Epitaxy (MBE) is a highly precise thin-film deposition technique used for the growth of single-crystal semiconductor layers under ultra-high vacuum conditions. By enabling atomic-scale control over composition and thickness, MBE has become an indispensable tool in the fabrication of advanced electronic and optoelectronic devices, including high-speed transistors, quantum wells, quantum dots, superlattices, and laser diodes.

Keywords: Molecular Beam Epitaxy (MBE), ultra-high vacuum, semiconductor heterostructures, thin-film growth, atomic layer control, RHEED, quantum wells, quantum dots, III–V compounds, wide bandgap materials, nanotechnology, optoelectronic devices, crystal growth, surface analysis, epitaxial layers.

Molecular beam epitaxy (MBE) is a process for producing epitaxial films by concentrating molecular beams on a substrate in a vacuum. The source of the molecular beams is a semiconductor material, usually silicon. The material is evaporated as a result of the action of an electron beam directed at the semiconductor or as a result of direct heating of the silicon wafer with an electric current. In the latter case, the sample (source) does not melt, but sublimation and transfer of the substance to the substrate occur.

The most important requirements for molecular sources are: high purity of the generated molecular beams; high purity of the source surface; stable evaporation rate in the operating mode; large supply of working substance; the ability to heat the evaporated substance over a wide temperature range.



The MBE process occurs in an ultra-high vacuum environment at a pressure of 1.33×10^{-6} to 1.33×10^{-8} Pa and at temperatures ranging from $400-800^{\circ}$ C. Under these conditions, the epitaxial layer growth rate is 0.01-0.03 µm/min, which is comparable to the growth rate observed in vapor-phase epitaxy. Furthermore, molecular beam epitaxy (MBE) offers several advantages over vapor-phase epitaxy, including:

- 1. The relatively lower processing temperature in MBE reduces impurity diffusion from the substrate and minimizes unintentional alloying.
- 2. The resulting MBE-grown layer exhibits high intrinsic resistivity due to the low probability of foreign impurity incorporation from the vacuum chamber onto the substrate.
- 3. The absence of intermediate chemical reactions and diffusion effects, combined with the low probability of particle collisions in high vacuum, allows precise control of the MBE process by adjusting source parameters such as material temperature and evaporation time.

The film growth process begins with the formation of atomic clusters at various points on the substrate surface where the incident beam atoms arrive. The lateral dimensions of these clusters are typically on the order of tens of angstroms. During the process, both the number and size of these clusters increase, eventually merging to form the main film layer. As a result, the initial continuous film typically forms at a minimum thickness of about 20–100 Å and is not monoatomic. This implies that the sources of defects in the film may stem from pre-existing imperfections in the nucleation stage as well as from defects introduced during the coalescence of growing embryos [1-3].

One of the key challenges in obtaining high-quality monocrystalline films is achieving uniformly distributed, unidirectionally oriented nuclei across the substrate. Even slight misorientation of the nuclei can significantly increase the defect concentration. Research has shown that there exists a specific epitaxial



temperature at which unidirectional nuclei form, and this temperature depends on a wide range of parameters grouped into three main categories:

- 1. Parameters describing the properties of atomic beams chemical composition, density, energy of incident particles, and beam geometry.
- 2. Parameters characterizing the substrate surface cleanliness, degree of structural perfection, orientation with respect to the molecular beam, and the substrate's chemical, physicochemical, and physical properties.
- 3. Parameters describing the technological process substrate temperature, concentration and nature of atmospheric impurities above the substrate, vacuum level, and duration of technological operations.

When an atom from the beam interacts with an atom on the surface, it can be captured by the substrate surface—this process is known as adsorption. Adsorption is classified into chemisorption and physical adsorption. In chemisorption, the interaction energy is on the order of one electron volt per atom, comparable to the energy of a chemical reaction [4-5]. Physical adsorption, on the other hand, results from weak van der Waals interactions between the beam atoms and the substrate atoms. An adsorbed atom, like a mobile particle in an excited state, diffuses across the substrate surface, transitioning from one potential well to another. Eventually, it may remain in one of these wells, interact with other atoms to form stable surface complexes (clusters), or desorb from the surface. The probability that an incident atom will be retained on the surface is characterized by the condensation coefficient, defined as the ratio of the number of atoms that condense on the surface to the total number of atoms incident on it. In addition to the condensation coefficient, an important parameter that characterizes the surface's ability to adsorb atoms from the atmosphere is the accommodation coefficient. Let an ideal monoatomic gas with temperature T1 and particle energy



If the atom is immediately reflected after the collision, the average energy gain is usually very small, meaning that the reflected atoms do not reach thermal equilibrium with the surface atoms. The average energy of the desorbed atom.

This coefficient describes the average fraction of energy exchanged between the incident beam atoms and the substrate in a single collision. If some atoms remain on the surface after adsorption, achieve thermal equilibrium with the substrate atoms [6-9].

The substrate surface temperature is generally lower than the average atmospheric temperature. The accommodation coefficient depends on the physical nature and mass of the interacting atoms; if their masses are comparable, the retained atom loses its energy through several substrate atom vibrations.

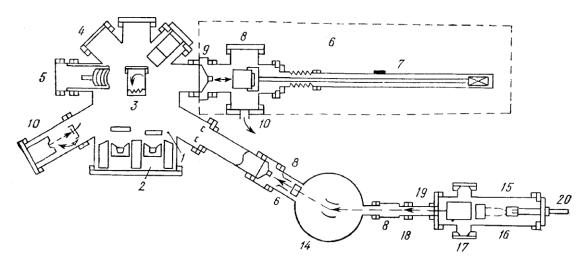


Figure 3.3. Molecular Beam Epitaxy (MBE) System

The process temperature is controlled using various methods, including thermocouples, infrared sensors, and optical parameters. To clean the sample surface, a low-power inert gas ion beam is used, sourced from an ion gun. The structure and purity of both the original substrate and the resulting layer are meticulously monitored using analytical instrumentation. For example, Auger spectroscopy, with a sensitivity of approximately 10^{12} atoms/cm², is employed to determine surface cleanliness and elemental composition. Crystallographic analysis of the substrate and deposited films is carried out via electron diffraction.



An electron beam directed at the substrate at an angle close to 1° generates an electron diffraction pattern, which can be used to determine unit cell parameters, analyze growth structures formed during layer deposition, and accordingly adjust the process parameters [10-14].

High-energy electron diffraction (with an accelerating voltage of 30–50 kV) is used to analyze grown layers, while low-energy electron diffraction (with accelerating voltages ranging from a few volts up to 1 kV) is applied to investigate surface structures. For chemical surface analysis, X-ray photoelectron spectroscopy is used, with a depth resolution of up to 5 nm and sensitivity down to 10^{13} atoms/cm².

In addition to the main technological operations (substrate surface cleaning, epitaxial deposition, and analysis of the deposited layers), auxiliary operations are also performed in the equipment, such as introducing the substrate into the deposition zone, transferring the substrate between chambers, and aligning it with respect to process and monitoring instruments. To minimize exposure of the high-vacuum system to air (even briefly or repeatedly), a load-lock system is employed. It includes two vacuum sorption pumps, a single ion pump with a capacity of 30 l/s, a magnetic mechanism for manipulating the loading rod, a loading window, and valve.

Unlike vapor-phase epitaxy, the use of MBE does not require special safety measures. The MBE method is considered highly promising for the fabrication of high-frequency and optoelectronic devices. Molecular Beam Epitaxy (MBE) is an advanced technology that enables the atomic-level controlled growth of semiconductor materials. This technique allows the formation of high-quality, defect-free, and compositionally uniform crystalline layers, which are critical for modern electronics and optoelectronics — including high-speed transistors, quantum wells and quantum dots, superlattices, lasers, and high-efficiency solar cells [15-20].



MBE technology offers several key advantages:

- Atomic-level precision: The thickness and composition of each layer can be controlled at the atomic scale.
- High purity: The growth process is carried out under ultra-high vacuum, significantly reducing the risk of contamination and ensuring extremely pure layers.
- Versatility: It enables the use of various materials, including III–V group semiconductors, oxides, and organic semiconductors.
- Real-time monitoring: Growth can be monitored in real-time using techniques such as Reflection High-Energy Electron Diffraction (RHEED).

However, MBE also has some limitations:

- Low growth rate: Typically, the growth rate is only a few microns per hour, which slows down the production process.
- High cost: Due to the complexity of the equipment and the requirement for ultra-high vacuum conditions, MBE is an expensive technology.
- Limited production scale: The low growth rate and high cost mean that MBE is primarily used for research and the development of specialized devices.

Conclusion:

In summary, Molecular Beam Epitaxy (MBE) plays a crucial role in fields where high precision and material purity are required — especially in nanoelectronics, quantum technologies, and advanced optoelectronic device fabrication. Its capabilities are widely utilized in scientific research and the development of next-generation technologies.

The previous sections have provided a detailed overview of the theoretical foundations of MBE, the associated equipment, growth parameters, and the properties of the resulting layers. MBE enables the atomic-scale fabrication of epitaxial layers by directing atomic or molecular beams onto a substrate in an ultrahigh vacuum environment. The method encompasses substrate preparation,



material evaporation from sources, real-time process monitoring using RHEED, and precise determination of growth rate and chemical composition. As outlined, key parameters such as the temperature of source heaters, pressure, substrate temperature, and molecular beam flux density directly influence the growth quality. Under optimal conditions, III–V semiconductor heterostructures (e.g., GaAs/AlGaAs, InP/InGaAs) exhibit extremely low crystallographic defect densities, atomic-scale thickness uniformity, and surface smoothness. These features make MBE a leading technology for producing high-frequency transistors, laser diodes, and quantum dots in advanced optoelectronic and microelectronic devices [20-24].

Furthermore, it is noted that high-quality wide-bandgap semiconductor layers such as gallium nitride (GaN), aluminum nitride (AlN), and oxides (ZnO, MgO) can also be synthesized using MBE. These materials, with properties such as wide bandgap, high thermal stability, and resistance to high-power operation, are advantageous in applications ranging from ultraviolet laser detectors to high-temperature and high-power electronics. These capabilities position MBE not only as a laboratory tool but also as a productive industrial technology. The challenges of the process include the high cost of MBE systems, the limited growth rate (a few microns per hour), and technical difficulties in achieving uniform layers over large areas. Nevertheless, ongoing research into creating nanometer-precision layers, optimizing heterostructure interfaces, and minimizing defects continues to improve the process's efficiency.

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