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# Summary of High Throughput Methods for Study of Thin Film Alloys

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**Abstract.** In the fields of semiconductor and electronics, fine processing at the micro and nanoscale is crucial. Thin film materials are an important part of this fine processing and their small molecular structure, ranging from microns to nanometers, is directly linked to achieving high throughput. Breakthroughs in thin film materials have accelerated research on high throughput systems and ultimately enabled mass production.

**Keywords:** Thin Film Materials; High-throughput Techniques; Ta-Ti Alloys.

## 1. Introduction

In the fields of chips and electronics, fine and precise processing is essential. Thin film materials play a crucial role in achieving the necessary level of precision. The molecular structure of thin film materials, which can be as small as micrometers or even nanometers, is directly related to achieving high throughput. Breakthroughs in thin film materials have also accelerated the research on high-throughput systems and enabled mass production.

Describe more general and systematic methods for High-Throughput Methods of Thin Films (materials preparation, data mining) for the Discovery of materials and the applications such as in solar cells and superconductors.

This paper summarizes three articles related to thin film materials and high-throughput techniques. The first article, "A combinatorial passivation study of Ta-Ti alloys," focuses on using the kinetics of anodic oxide formation to analyze Ta-Ti alloys' properties. The second article, "Combinatorial study of phase transformation characteristics of a Ti-Ni-Pd shape memory thin film composition spread in view of microactuator applications," studies the phase transformation characteristics of Ti-Ni-Pd shape memory thin film composite materials. The third article, "Combinatorial fabrication and high-throughput characterization of a Ti-Ni-Cu shape memory thin film composition spread," analyzes the phase transformation characteristics of Ti-Ni-Cu shape memory thin film materials.

## 2. Literature References

### 2.1. Article 1: A Combinatorial Passivation Study of Ta-Ti alloys

In this article, the authors used the kinetics of anodic oxide formation to analyze the properties of Ta-Ti alloys. Droplet cell scanning is used in this experiment. The local anodization of Ta-Ti alloys was carried out using a scanning droplet cell (SDC), which featured a capillary-based microelectrochemical design with a three-electrode configuration. To construct the cell, a borosilicate capillary with a diameter of 2.5 mm was carefully pulled using a Narishige puller (PC-10). This capillary serves as the outer body of the cell. A micro-grinder (Narishige EG-400) was employed to create a tip with a diameter of 200 µm. The reference electrode utilized in the cell was a capillary l-AuHg/Hg2(CH3COO)2/NaCH3COO reference electrode, with a 1 mm outer diameter and a 100 µm tip diameter. For the counter electrode, a 1 mm wide Au stripe was wrapped around the reference electrode capillary and inserted into the main body capillary. All the components of the SDC were meticulously assembled within a plastic block, following the procedures outlined in previous reports.

To ensure a proper seal, a silicone gasket was generated at the tip of the cell by immersing it in liquid silicone and drying it using a nitrogen flow. During the experiments, the tip of the cell was pressed against the surface of interest to ensure consistent wetting of the Ta-Ti alloys. This direct contact prevented any electrolyte-air interaction and effectively prevented volume expansion of the electrolyte droplet due to electrocapillarity, ensuring accurate measurements. The experiment used an automated scanning droplet cell for high-throughput screening. Cyclic voltammetry increased anodic polarization, and electrochemical impedance spectroscopy was performed. This method yielded a complete set of oxide parameters, including film-forming factor, dielectric constant, oxide-specific resistance, flat-band potential, and donor density. These properties are directly related to the mother material's microstructure. A mixture of Ta and Ti can form a stable phase for Ta concentrations >83 at.% at 400°C. The Ta-Ti phase diagram shows immiscibility and a low Ta phase for very low Ta contents. Co-deposition of Ta and Ti at low temperatures can produce thin metallic films with deviations from the bulk phase diagram. The microstructure of Ta-Ti alloys was examined using SEM, revealing different grain types and their evolution with Ti content. The addition of Ti alters the microstructure, resulting in the disappearance of certain grain types and the formation of new ones. The crystallographic orientations of the alloys, as measured by XRD, confirm the observed microstructural changes. Potentiodynamic oxide formation experiments were conducted, and the current density plateaus were analyzed to determine the oxide formation factor. Impedance measurements were also performed to characterize the anodic oxides. The oxide formation factor, dielectric constant, and electrical resistivity were mapped across the Ta-Ti composition range, revealing trends and variations with Ti content. The properties of the anodic oxides on pure Ta and Ti were used as reference points for comparison.

### 2.2. Article 2: Combinatorial Study of Phase Transformation Characteristics of a Ti-Ni-Pd Shape Memory Thin Film Composition Spread in View of Microactuator Applications

In this article, the authors studied the phase transformation characteristics of Ti-Ni-Pd shape memory thin film composite materials. The Ti-Ni-Pd samples were prepared using an ultra-high-vacuum magnetron sputtering deposition system, and the film composition was annealed in situ between 500 - 800 °C. Energy dispersive X-ray analysis (EDX) and X-ray diffraction measurements (XRD) were used for high-throughput characterization of the component diffusion. The authors found that a reversible phase transformation can be observed within the measurement range of 40 - 250 °C when the Ti content is between 50-59 at.%. For Ti-rich films, the Ti2Ni and Ti2Pd precipitates suppress the reversible phase transformation. The transformation temperature and hysteresis were determined by R(T) measurements. Compared with B2-R-B19, the B2-B19 transformation temperature increases with increasing Pd content, and the hysteresis decreases significantly, consistent with published data. For components with low Pd content (< 7-12 at.%, depending on Ti content), two-stage B2-R-B19 transformation is observed. The high Pd content component shows a single-stage B2-B19 transformation. The hysteresis linearly increases with increasing Ti content in the B2-B19 transformation region, and the transformation temperature linearly decreases.

### 2.3. Article 3: Combinatorial Fabrication and High-Throughput Characterization of a Ti-Ni-Cu Shape Memory Thin Film Composition Spread

This paper investigates the phase transition properties of Ti-Ni-Cu shape memory films prepared in a compositionally graded manner. A combination of high vacuum magnetron sputtering deposition system is used to deposit Ti, Ni, and Cu alternating wedge-shaped layers on a thermally oxidized silicon substrate, followed by in situ annealing at 500°C for 1 hour. The composition regions of the ternary phase diagram where the thermoelastic transformation occurs are determined through automated temperature-dependent resistance measurements, energy-dispersive X-ray analysis, and X-ray diffraction measurements. Transition temperatures and hysteresis are determined using resistance measurements. A wide transition region is observed within the compositional range. For compositions rich in Ni, a two-stage B2→R→B19' transformation is observed. In the $Ti_{51}Ni_{49-x}Cu_x$ (at.%) compositions, a single-stage transition (B2→B19') is observed when the Cu content is <6.5

at.%, while a single-stage transition (B2→B19) is observed when the Cu content is >14 at.%. A two-stage transition (B2→B19→B19') is observed in the intermediate composition range. The experimental results agree with the literature's description of the relationship between Cu content and hysteresis.

The study also explores the microstructure and mechanical properties of Ti-Ni-Cu shape memory films. Scanning electron microscopy and transmission electron microscopy reveal uniform surface morphology and dense crystalline structure in the deposited films. Mechanical testing shows that the Ti-Ni-Cu films exhibit good performance in the shape memory effect.

Further experimental investigations analyze the kinetic characteristics of phase transitions in Ti-Ni-Cu films. Measurements of transition rates and hysteresis provide insights into reaction speed and energy dissipation during the phase transition process. The results indicate that the transition rate increases significantly, and hysteresis decreases with increasing Cu content. These findings are crucial for designing and controlling the performance and response of Ti-Ni-Cu shape memory films.

In summary, this study provides an in-depth exploration of the phase transition properties, microstructure, and mechanical properties of Ti-Ni-Cu shape memory films. By understanding and optimizing the characteristics of these films, we can provide more theoretical and practical foundations for the development and application of shape memory alloys, thus driving further advancements in related technologies.

## 3. Conclusion

In conclusion, the use of thin film materials has revolutionized the fields of chips and electronics by enabling fine and precise processing and high throughput. The three articles summarized in this paper provide valuable insights into the properties and phase transformation characteristics of Ti-Ni-Pd and Ti-Ni-Cu shape memory thin film composite materials and Ta-Ti alloys. The authors utilized various high-throughput techniques, such as automated scanning droplet cells, energy dispersive X-ray analysis, and X-ray diffraction measurements, to study the molecular structure and properties of these materials. These studies will undoubtedly contribute to the development of new and improved thin film materials and high-throughput systems, paving the way for future technological advancements in the field of chips and electronics.

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