



Article Deposition of Nb-Si-C Thin Films by Radio Frequency Magnetron Sputtering

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Abstract: Nb-Si-C thin films were deposited onto Si(001) substrates by radio frequency (RF) magnetron sputtering using individual Nb, Si, and C targets. The effects of varying the sputtering power on the phase composition of the new thin films were studied. The structure, chemical components, and morphology of the thin films were characterized by X-ray diffraction, X-ray photoelectron spectroscopy, scanning electron microscopy, and atomic force microscopy. The experimental results and first-principles calculations indicate that a new MAX phase (Nb₄SiC₃) can be synthesized at a sputtering power of 65 W. The four-point probe test showed that the resistivity of the film containing Nb₄SiC₃ phase was 0.99 μ Ω·m. A nano-indentation test showed that the hardness of the film containing Nb₄SiC₃ phase was 15 GPa, and the elastic modulus was 200 GPa.

Keywords: Nb-Si-C system; radio frequency magnetron sputtering; MAX phase; Nb₄SiC₃



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1. Introduction

The group of ternary layered ceramics known as the MAX phases not only have the electrical conductivity and heat conduction of metals but also the high elastic modulus, high temperature resistance, low thermal expansion coefficient, and the oxidation and corrosion resistance of ceramics [1–3]. Bulk MAX phases are used to make high-temperature components, foil bearings, burner nozzles, rubber molds, and metal-cutting tools [4]. MAX phase films are used for nuclear fuel cladding, high-temperature-resistant coatings, electrical components, and in other fields [5].

MAX phases have the structure $M_{n+1}AX_n$, where n = 1-3, M is an early transition metal, A is an A-group element, and X is either C or N. The MAX phase materials are a group of 60+ ternary carbides and nitrides [6]. They have a layered structure with hexagonal symmetry (P63/mmc). In the MAX phases, near-close-packed layers of transition-metal carbide and/or nitride are interleaved with layers of a pure A-group. In the M₂AX phases, A-layers are separated by two M-layers; in the M₃AX₂ phases, A-layers are separated by three M-layers; and in the M₄AX₃ phases, A-layers are separated by four M-layers [7].

Thin-film deposition of the MAX phases has been studied for many years, with physical vapor deposition and chemical vapor deposition as two main approaches. In recent years, sputtering has become the most popular method for synthesis of MAX phase thin films. There are two different methods for sputtering: from individual M, A, and C targets or from compound targets. The former is mainly used in the laboratory because the effects of different constituent elements on the structure and properties of the final products can be investigated easily and efficiently. The latter uses a single compound target for sputtering; the preparation process is relatively simple and has good repeatability, but it often leads to the problem of large deviation between the product and the chemical composition of the target material.

To date, many MAX phase thin films have been synthesized, particularly in the Ti-Si-C [8–10], Ti-Al-N [11–14], Ti-Al-C [15–17], Ti-Ge-C [18], Cr-Al-C [19,20], V-Al-C [21], and Nb-Al-C [22] systems; however, there have been few reports on the preparation of the Nb-Si-C system. Researchers have prepared Nb-Si-C thin films by magnetron sputtering from individual Nb, Si, and C targets and obtained a mixture of NbC, SiC, and NbSi phases. The films exhibit nanocrystalline and amorphous structures. The segregation of Si at the NbC grain boundary will hinder the diffusion of Nb and C [23,24]. They also found that the change of silicon content in the film has a great effect on the microstructure and properties of the film [25].

In recent years, many researchers have used computational materials science to predict the stability of MAX phase and their properties. The most widely used of these is density functional theory (DFT) [26–29]. According to DFT, in the Nb-Si-C system, only Nb₄SiC₃ is stable [30]. The theoretical existence of Nb₄SiC₃ is a metal and exhibits covalent nature. Moreover, the hardness of Nb₄SiC₃ is much higher than Nb₄AlC₃; meanwhile, it is more ductile than Nb₄AlC₃. Its high hardness and bulk modulus are due to the covalent bonding in Nb₄SiC₃ [31]. To sum up, the Nb-Si-C system may have excellent electrical, optical, and mechanical properties. The Nb-Si-C film has the potential to be a material with low electrical resistance and high wear resistance [32]. It also has the potential to be synthesized by typical methods. By adjusting the different sputtering processes, the composition of each element in Nb-Si-C thin film can be adjusted; the film with better performance can then be prepared, and it is possible to prepare a new MAX phase of Nb-Si-C system. Researchers often employ the following two process adjustments: the first is to adjust the sputtering power; the second is to adjust the area ratio of the target material to be similar to the stoichiometric ratio of the MAX phase.

The purpose of this research was to deposit Nb-Si-C thin films from three separate Nb, Si, and C targets using radio frequency magnetron sputtering at low temperatures through different power. The microstructure, composition, and properties of the deposited Nb-Si-C thin films were investigated by X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), scanning electron microscopy (SEM), energy dispersive spectrometer (EDS), atomic force microscopy (AFM), nano-indentation, and four-point-probe resistance tester. Another purpose of the research was to find sputtering technology that could prepare a new MAX phase.

2. Materials and Methods

Nb-Si-C films were deposited by radio frequency magnetron sputtering using (the JGP450-PECVD200 magnetron sputtering apparatus, SKY, Shenyang, China) from three separate targets at 25 °C. The working gas of the deposition was Ar gas. Single-crystalline Si(001) wafers were selected as substrate for deposition of Nb-Si-C films. Their size was 10 mm \times 10 mm \times 1.5 mm. Substrate of Si(001) was cleaned in acetone, ethanol, and deionized water for 10 min to remove dust and impurities from the surface. The cleaned substrate was dried to keep the surface clean during the process, and the substrate was placed into a drying dish.

A slice of Si (99.99%) and three slices of graphite (99.99%) targets were stuck on a circular slice of Nb (99.95%) in the area ratio of 1(Si):3(C):5(Nb). We hoped that the percentage of elements in the film after sputtering would be similar to that of the Nb₄SiC₃ MAX phase. The Si target was 10 mm \times 5 mm \times 1.5 mm, the C target was 10 mm \times 5 mm \times 1 mm, and the Nb target was 12 mm in radius and 3 mm thick. The distance between the substrates and the targets was 60 mm. The vacuum chamber was pumped to a pressure of 3.0×10^{-5} Pa. Then, a certain amount of Ar gas was introduced to control the cavity pressure at 1.0 Pa. In order to remove contaminants from the substrate, it was presputtered by Ar ions at a bias voltage of -200 V for 15 min. The working pressure of Ar (99.999%) was 2.4 Pa and the flow rate was 25 sccm. The bias voltage was -100 V, as shown in Table 1.

Si/C/Nb	Ar Gas Flow	Sputtering	Vacuum Degree	Base Bias	
Area Ratio	Rate (sccm)	Pressure (Pa)	(Pa)	(v)	
1:3:5	25	2.4	$3 imes 10^{-5}$	-100	

Table 1. Fixed parameters in sputtering deposition.

The binding force of the elements varied with sputtering power. By adjusting the sputtering power of Nb target and Si target, Nb-Si-C composite films with very different structures and properties were prepared. The researchers also found that the fiber structure of the film was very sensitive to changes in Si content [25]. Some scholars changed the content of silicon in the deposited film by the number of Si plates affixed to the niobium target [32].

To investigate the impact of sputtering power, Nb-Si-C thin films specimens were synthesized at five different sputtering powers: 65, 70, 75, 80, and 100 W. The sputtering time for all specimens was 60 min. The sputtering time and sputtering power for each group of parameters (from a to e) are shown in Table 2.

 Table 2. Process parameters used in sputter deposition.

Process Parameters	а	b	с	d	e
Sputtering time (min)	60	60	60	60	60
Sputtering Power (W)	65	70	75	80	100

The structure of the thin films was characterized by X-ray diffraction (XRD, Panalytical, Almelo, The Netherlands) with a CuK α radiation source ($\lambda = 0.14505$). The measurements were taken over a detection range of θ –2 θ with a step of 0.02°. The acceleration voltage was 40 kV, and the current was 40 mA. The composition and chemical states of the thin films were analyzed by X-ray photoelectron spectroscopy (XPS, Thermo Fisher Scientific, Waltham, MA, USA) with a AlK α source.

The microstructure of the films was observed with scanning electron microscopy (SEM, Thermo Fisher Scientific, Waltham, MA, USA) and atomic force microscopy (AFM, Bruker, Karlsruhe, Germany). Energy dispersive spectrometer (EDS, Thermo Fisher Scientific, Waltham, MA, USA) was used to measure the chemical composition of the films, the acceleration voltage was 20kV. The electrical resistivity of the thin films was tested with a four-point probe resistance tester. Nano hardness and elastic modulus of the films were measured by nano-indentation. The test adopted continuous stiffness measurement technology (CSM) with a Berkovich indenter, (Agilent Technologies, Palo Alto, CA, USA). The indenter was pressed to a depth of 200 nm with a load time of 10 s. In order to reduce the error, we carried out the process five times at different parts on each film and then took the average value of the five measurements as the hardness of each film.

3. Results and Discussion

Figure 1 shows the X-ray diffraction results of the five deposited thin films (a to e) from Nb, Si, and C targets onto Si(100) substrates with a sputtering power from 65–100 W and a sputtering time of 60 min.

For film a, there are four diffraction peaks in the figure, including SiC peaks at 35.2° , 61.0° , 72.5° , and an undesignated diffraction peak at 42.3° . According to the analysis of the three targets, it is also possible that these diffraction peaks represent a new Nb-Si-C ternary compound. To verify this hypothesis, we refer to the research literature on the calculation of the Nb-Si-C MAX phase, which used density functional theory with generalized gradients to simulate the XRD patterns of the Nb₄SiC₃ MAX phase [31]. After comparison with this experiment's XRD pattern, it was found that the three strongest peaks in the experimental were in good agreement with the simulated data (the vertical marks), so it can be assumed that there was a Nb₄SiC₃ MAX phase in film a. For films b to e, only two kinds of diffraction

peaks could be found, corresponding to NbC and SiC. From the diffraction results, it can be observed that when the sputtering power is higher than 70 W, Nb-Si-C system ternary compounds are not formed.



Figure 1. X-ray diffraction patterns of the five deposited thin films (a to e). The vertical marks are the simulated XRD peaks of Nb_4SiC_3 phase. The three strongest peaks in the experiment are in good agreement with the simulated data.

Table 3 shows the EDS composition analysis results of the thin films (from a to e). It can be seen that with the increase of sputtering power, the atomic percentage of C increases continuously, from 30% to 44%. The atomic content of Si decreases continuously, from 25% to 15%, while the atomic content of Nb fluctuates within a certain range.

Sputtering Power (W)	C (at.%)	Si (at.%)	Nb (at.%)
65 (a)	30 ± 1.6	25 ± 1.7	45 ± 0.5
70 (b)	36 ± 1.8	23 ± 1.3	41 ± 0.6
75 (c)	42 ± 1.6	21 ± 1.6	37 ± 0.7
80 (d)	40 ± 1.8	18 ± 1.5	42 ± 0.5
100 (e)	44 ± 2.1	15 ± 1.7	41 ± 0.4

Table 3. EDS composition analysis results of the thin films (from a to e).

Combined with the previous analysis of the composition of the films, with the increase of sputtering power, the content of C element in the film increases gradually, and the number of Nb-C compounds in the coating increases. At this time, the Si element is difficult to insert into Nb-C compounds with strong bond energy, and it can be considered that the formation of Nb₄SiC₃ MAX is inhibited to some extent by the increase of Nb-C compounds.

X-ray photoelectron spectroscopy was used to investigate the undesignated diffraction peaks in film a. The data obtained were analyzed with XPSPEAK software (version 4.0, Hong Kong, China), and the narrow scan peaks of Nb 4d, Si 3p, and C 2p were fitted with different peaks. As shown in Figure 2, there are two peaks in Nb4d (206.8, 209.2 eV). The Nb-Si-C film correlation calculation indicates that some Nb is bonded to C, and the rest is bonded to Si. There is one peak in Si3p (106.4 eV), indicating Nb is bonded to Si. There is one peak in C2p (284.5 eV), indicating Nb is bonded to C.



Figure 2. X-ray photoelectron spectroscopy for film a.

These experimental results, combined with preliminary studies on Nb₄AC₃ MAX phases using density functional theory, indicate that the phase of the new thin film could be Nb₄SiC₃. Until now, there have been no reports on the preparation of Nb₄SiC₃ MAX phase.

The five deposited thin films (from a to e) were observed with a scanning electron microscope. Figure 3 shows that the surfaces of the experimentally synthesized films are dense, homogenous, and crack free; they are also observed to be polycrystal. Figure 4 shows a cross-sectional of film a; the thickness of the film was about 270 nm. Figure 5 shows the AFM 3D morphology of film a; the roughness value of the film is 1.68 nm.

The surface is smooth and the roughness is small, which indicates that the film has good wear resistance.



Figure 3. SEM images of the thin films deposited at 25 $^{\circ}$ C for 60 min with different power: (a) 65 W, (b) 70 W, (c) 75 W, (d) 80 W, and (e) 100 W.



Figure 4. Cross-sectional image of thin film a deposited at 25 °C for 60 min with 65 W.



Figure 5. The AFM 3D micrograph of the thin film a deposited at 25 °C for 60 min with 65 W. The roughness value of film a is 1.68 nm.

Electrical conductivity tests using the RTS-9 double-resistance four-probe test were carried out, and the electrical resistivity of the synthetic films a to e ranged from 0.79 to 2.2 $\mu\Omega$ ·m. As shown in Table 4, when the power was 65 W, the electrical resistivity of film a was 0.99 $\mu\Omega$ ·m. When the power is greater than 65 W (films from b to e), the electrical resistivity was in turn 1.95, 2.06, 1.89, and 2.20 $\mu\Omega$ ·m respectively. Analysis showed that the resistivity of film a was lower than that of other samples, which can indirectly prove that film a generated Nb₄SiC₃ MAX phase. This was also consistent with the relevant literature, which indicates that MAM phase was a good conductor of electricity and that the room

temperature resistivity generally ranged from 0.07 to 2 $\mu\Omega$ ·m. Many MAX materials have an even lower resistivity than titanium [33].

Sputtering Power (W)	Hardness (GPa)	Elastic Modulus (GPa)	Resistivity (μΩ∙m)
65 (a)	15 ± 1	200 ± 16	0.99
70 (b)	18 ± 1	215 ± 10	1.95
75 (c)	19 ± 1	200 ± 17	2.06
80 (d)	20 ± 1	220 ± 15	1.89
100 (e)	20 ± 2	215 ± 13	2.20

Table 4. Mechanical properties and electrical resistivity of the thin films.

Nano-hardness and elastic modulus of films deposited with different power were tested by a nano-indentation instrument. As shown in Table 4, when the power was 65 W, the nano-hardness and elastic modulus of the film were 15 and 200 GPa. When the power was greater than 65 W, the hardnesses of the films were from 18 to 20 GPa, and the elastic moduli were from 200 to 220 GPa. It can be seen from the nano-hardness test that when the power was 65 W, the hardness of the film was far less than that of the other films; the main reason could be the formation of Nb₄SiC₃ MAX phase in the film, as its hardness is far lower than the binary Nb-C ceramic phase. It is suggested in some literature that if the ratio of hardness to elastic modulus (H/E) is higher, the film can obtain higher wear resistance. According to the experimental data, film a has an H/E value of 0.075; the values of films b to e are 0.084, 0.095, 0.091, and 0.093, respectively. Based on this result, it indicates that among the five sputtering films, the wear resistance of film c is the highest, while that of film a is the lowest. By adjusting the sputtering power of Nb-Si-C film and changing the proportion of three elements, the film with the best wear resistance can be achieved.

As for the mechanical properties of Nb-Si-C thin films, some scholars believe that the hardness of Nb-Si-C thin films will decrease with the generation of more Si-C phase in the film and that the increase of the amorphous phase caused by Si in ternary films is also a way to reduce the hardness [32].

4. Conclusions

In conclusion, we synthesized Nb-Si-C thin films by radio frequency magnetron sputtering. The results show that the microstructure and properties of the films were closely related to the deposition power. When the deposition power was greater than 70 W, the deposited films were mainly NbC and SiC phases. When the deposition power was 65 W, a new ternary phase was formed in the thin film in addition to the NbC and SiC phases. Based on the analysis of the experiment and the comparison with the results of the structural calculation, we predict that the ternary Nb-Si-C compound might be Nb₄SiC₃ phase. The formation of ternary compounds is related to the content of C and Si in the sputtering process. Excessive C content will hinder the formation of ternary compounds.

According to the four-point probe test, Nb-Si-C thin films have relatively low resistivity. Moreover, they also have high hardness and elastic modulus. Based on the above properties, Nb-Si-C thin films can be used to make electrical contacts and thermal printing heads.

This study suggests that different sputtering power can be used to prepare Nb-Si-C thin films with different properties and that Nb_4SiC_3 phase can be prepared at lower power. Finally, we believe that single-phase Nb_4SiC_3 thin film can be prepared by proper sputtering technology. The preparation of single-phase Nb_4SiC_3 thin film and the evaluation of their properties should be further studied in future.

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