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Effect of Reactive Gas Flow Ratio on IC-PECVD Deposited a-SiC:H Thin Films

Tobias Frischmutha*, Michael Schneidera, Thomas Grilleb, Ulrich Schmida

aInstitute of Sensor and Actuator Systems, Vienna University of Technology, Floragasse 7/2, 1040 Vienna, Austria
bInfineon Technologies Austria AG, Siemensstraße 2, 9500 Villach, Austria

Abstract

Hydrogenated amorphous silicon carbide layers are deposited using an inductive-coupled plasma-enhanced chemical vapour deposition process. The nominal thickness of the thin films is 300 nm and the chemical composition ranges from carbon rich to pure Si films by varying the silane to methane ratio $\chi$. The compressive residual stress of the Si-C compound exhibits a maximum at $\chi = 0.45$. The deposition rate and the refractive index increase linearly with increasing $\chi$. Furthermore, Fourier transformed infrared spectroscopy shows a correlation of the Si-C vibration mode with the residual stress.

Keywords: Silicon carbide, residual stress, PECVD, MEMS, FTIR;

1. Introduction

Silicon Carbide (SiC) is an interesting and rigid material for high performance MEMS devices. Its mechanical robustness, as well as its high thermal and chemical resistivity makes it a promising material with great opportunities and challenges for applications in harsh environments [1]. SiC exists in different polytypes and modifications (i.e. mono-/polycrystalline, amorphous) [2] and is used in multiple applications as bulk material, as well as on thin film level [3, 4]. In order to realise advanced systems and devices (e.g. high temperature pressure sensors or radio frequency (RF) MEMS switches), the optimisation of thin film properties is of utmost importance.

* Corresponding author. Tel.: +43-1-58801-36647; fax: +43-1-58801-36698.
E-mail address: tobias.frischmuth@tuwien.ac.at
The current study presents a simple approach to tailor the properties (such as film stress and refractive index) of inductive-coupled plasma-enhanced chemical vapour deposited (IC-PECVD) hydrogenated amorphous SiC (a-SiC:H) thin films through variation of the silane (SiH₄) to methane (CH₄) gas flow ratio \( \chi \). The quality of the films and their chemical composition is validated using Fourier transformed infra-red spectroscopy (FTIR), showing the strong impact of \( \chi \) on the chemical binding state and exposing a clear correlation between \( \chi \), mechanical film stress and concentration of Si-C bonds.

2. Experimental Details

The thin films used for this study were deposited on 350 µm thick, double side polished 4” Si (100) wafers. The surface was cleaned with an EVG EV 300 megasonic wafer cleaner and the natural oxide layer was removed using a 5% buffered HF etching solvent prior to deposition. The a-SiC:H thin films were synthesised using an OXFORD INSTRUMENTS Plasmalab System 100 at a substrate holder temperature of 250°C and a chamber pressure of 6 mTorr. Inductive coupled plasma at 2000 W at a RF of 13.56 MHz was used as an ionization source. Layers were deposited at different SiH₄ to CH₄ ratios, while keeping the sum of SiH₄ and CH₄ flow rates at 20 sccm and the argon flow rate at 50 sccm. Deposition time was set to achieve nominal layer thicknesses of 300 nm. The thickness of the layer was measured with a Filmetrics F20 spectral reflectance meter. In addition, the film stress was determined using an E+H Metrology MX203-6-33 wafer bow measurement equipment. The FTIR spectra were recorded with a BRUKER TENSOR FTIR Spectrometer, measuring the IR absorbance at the centre of the wafer. The measured FTIR spectra were processed by subtracting the background and the Si-substrate reference spectra. Additionally, a polynomial baseline fit of the spectra was obtained and the absorption coefficient \( \alpha(\omega) \) calculated, following the Beer-Lambert law (1)

\[
\alpha(\omega) \cdot t = - \ln \left( \frac{I(\omega)}{I_0(\omega)} \right),
\]

where \( t \) is the thickness of the layer and \( I(\omega) \) and \( I_0(\omega) \) are the intensities of the incident and the transmitting radiation, respectively. Finally, the deconvolution of certain vibration modes is achieved by using a combination of Lorentzian and Gaussian functions which yields good fitting results.

3. Results and Discussion

Mechanical stress of thin films has a huge impact on the dynamic and the static behaviour of MEMS devices. Tailoring the intrinsic film stress in the “as-deposited” state of the layer provides the opportunity to optimise the performance of the whole system. Furthermore, the impact of the gas flow variation on certain thin film parameters, mainly residual stress, but also refractive index in the “as-deposited” state and the deposition rate of the process is measured and qualitatively discussed, taking the FTIR spectra into account.

3.1. Influence of \( \chi \) on stress, deposition rate and refractive index

The resulting impact of the gas flow variation on the mechanical stress and deposition rate is yielded in Fig. 1a. The compressive film stress exhibits a local maximum of -752 MPa at flow rates of 13.75 sccm CH₄ and 6.25 sccm SiH₄ (representing a ratio of 0.45) while decreasing towards tensile at higher, as well as lower \( \chi \) values. The lower film stress of the a-SiC:H layers due to a higher Si concentration is in good agreement to data observed from RF-PECVD deposited a-SiC:H thin films [5]. On the other hand, the lower stress of thin films deposited at higher CH₄ flow rate is interesting and will be further analysed, as a-C:H thin films tend to have an even higher compressive “as-deposited” residual stress [6]. The deposition rate increases rather linearly from 7.5 to 25 nm·min⁻¹ with increasing \( \chi \). This tendency can be attributed to the higher bond-dissociation energy of CH₄ compared to SiH₄ [7]. Based on preliminary studies it is reasonable to assume, that the films deposited at \( \chi = 0.45 \) exhibit stoichiometric composition, which correlates well with the observed maximum in film stress. As shown in Fig. 1b,
the refractive index increases from 1.95 to 2.49 linearly with $\chi$ due to the higher Si content of the deposited thin film.

3.2. Influence of $\chi$ on the chemical composition

These considerations are validated using FTIR measurements, as illustrated in Fig. 2a, based on vibration modes representing the investigated $\chi$ range, showing a strong impact of $\chi$ on the shape of the resulting spectra. To analyse the influence of $\chi$ on certain vibration modes, the deconvolution of the main peak ranging from 1200-400 cm$^{-1}$ and containing Si-Si stretching, Si-C stretching and Si-C-H$_2$ wagging modes is shown in Fig. 2b for selected $\chi$ values. The Si-C stretching vibration is the essential mode of the deconvoluted vibration compound and has its maximum at $\chi = 0.43$. On the other hand, the hydrogen containing Si-C-H$_2$ wagging is more distinct at a CH$_4$ rich deposition processes, as is the Si-Si stretching mode for layers synthesised at an increased SiH$_4$ ratio. To define these coherences, the concentration of the bonds is calculated by integrating the absorption coefficient of the band [8], which results in the characteristics of the deconvoluted peak areas as presented in Fig. 3a. With increasing $\chi$, the Si-C-H$_2$ peak decreases, whereas the Si-Si mode is negligible at enhanced methane flow rates, but strongly increases at $\chi > 0.55$. The integrated Si-C vibration mode correlates well with the residual stress, showing a maximum between flow ratios.

![Fig. 1](image1.png)

**Fig. 1** (a) Influence of $\chi$ on film stress and deposition rate; (b) Dependency of the refractive index at $\lambda = 632.8$ nm on $\chi$.

![Fig. 2](image2.png)

**Fig. 2** (a) FTIR spectra of a-SiC:H thin films deposited at selected $\chi$; (b) Deconvolution of the main peak, showing the Si-Si stretching, the Si-C stretching, and the Si-C-H$_2$ wagging mode.
of 0.4 to 0.5, thus supporting the assumption of a film composition which is at least close to stoichiometry. Additionally, the dependency of $\chi$ on hydrogen containing bond density is shown in Fig. 3b, yielding an increase of Si-H and a decrease of C-H at higher $\chi$ values, proving the assumptions introduced above.

![Graph](image-url)

Fig. 3 (a) Peak area characteristics of the deconvoluted FTIR-modes as a function of $\chi$; (b) Dependency of the amount of Si-H and C-H vibration modes on increasing $\chi$.

### 4. Conclusion

Variation of SiH$_4$/CH$_4$ ratio on “as-deposited” a-SiC:H layers was carried out, allowing a wide range optimisation of thin film properties. The residual stress yields a compressive maximum of -752 MPa which correlates well with the maximum of Si-C bonds, determined from the FTIR spectra. On the other hand, deposition rate, refractive index and amount of Si-H vibrations increase with higher SiH$_4$ content, whereas the amount of C-H modes decreases.

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### References


