A10.83Sc0.17N Contour-Mode Resonators with Electromechanical Coupling in Excess of 4.5%

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Al$_{0.83}$Sc$_{0.17}$N Contour Mode Resonators with electromechanical coupling in excess of 4.5%

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Abstract—In this paper we demonstrate the fabrication of contour mode resonators (CMRs) with Al$_{0.83}$Sc$_{0.17}$N as piezoelectric layer. Moreover, we assess the electromechanical coupling and the maximum achieved quality factor from 150 MHz to 500 MHz. In comparison to pure aluminum nitride (AlN) CMRs, our results show electromechanical coupling coefficients of more than a 2× factor higher at around 200 MHz. The highest quality factor is measured on a CMR operating at 388 MHz and is in excess of 1600. From the characterization of devices operating at different frequencies material parameters of the Al$_{0.83}$Sc$_{0.17}$N are extracted such as the stiffness constant, the relative permittivity and the piezoelectric constant. In particular, the reported $d_{31}$ piezoelectric constant is equal to -3.9 pm/V. This represents a 2.25× improvement when compared to pure AlN. Finally, we report the first temperature compensation experimental results for Al$_{0.83}$Sc$_{0.17}$N CMRs. Our results show that about 1.5 μm of sputtered oxide, deposited on top of released resonator, allows near zero TCF for CMRs operating up to 500 MHz.

Index Terms—Contour mode resonators, aluminum scandium nitride, quality factor, electromechanical coupling, material properties, temperature compensation.

I. INTRODUCTION

In timing and filtering applications MicroElectroMechanical Systems (MEMS) based solutions are gathering attention for their small form factors and compatibility with CMOS technology. In particular, CMRs have been widely investigated for the possibility to set the operating frequency by layout technology. In particular, CMRs have been widely investigated for their small form factors and compatibility with CMOS (CMOS) based solutions. Moreover, the strong anisotropy of the material makes the fabrication very challenging and not compatible with standard IC processes.

On the other hand, alloying of the aluminum nitride (AlN) thin film has been explored for the advantage of being CMOS compatible. Moderate doping of the Al target with chrome, erbium, and tantalum [18-20] have proven to provide piezoelectric response enhancement up to 100%. However, the most promising doping is with scandium (Sc). 50% Sc replacement in the Al target led to a piezoelectric response improvement of around a factor of 4 [21]. This increase in electromechanical coupling is justified by the fact that Sc doping causes the Young’s modulus of the Wurtzite structure to decrease, while the dielectric and piezoelectric constants increase [22].

AlScN has been used as piezoelectric layer to fabricate FBARs showing up to 100% increase in electromechanical coupling as the Sc doping is increased to 15% [23]. A low-loss 3 GHz surface acoustic wave (SAW) resonator showed relatively high $k^2$ of 5% in 46% doped AlScN [24]. Laterally vibrating Lamb wave resonators with up to 40% Sc doping achieved a 5x improvement in the electromechanical coupling with respect to pure AlN [25, 26].

In this study, we demonstrate 17.25% metal atom ratio AlScN one-port CMRs and we provide an extensive
characterization of both material properties and device characteristics. In order to investigate if anchor loss is the main dissipation mechanism, similarly to AlN, devices with different anchor width (W_a) are fabricated. Moreover, devices with different pitches are fabricated to assess the frequency variation as a function of the electrode pitches. Finally, we show that the same TCF (temperature coefficient of frequency variation) compensation technique used in AlN resonators (adding an oxide layer to the resonator) can be successfully implemented in AlScN.

II. METHODS

A. Device and fabrication

The devices fabricated in this work are all 1-port CMRs and the lateral field excitation (LFE) configuration is employed to electrically excite lateral motion in the resonators. In LFE, the bottom metal is a plate at floating potential, while the top metal is made of interdigitated (IDT) electrodes. The vertical component of the produced electric field is converted into lateral strain, in the direction of the resonator’s width, by means of the piezoelectric coefficient d31.

An analytical formulation for the CMRs’ resonance frequency is given by (1),

\[ f_r = \frac{v_{s0}}{\lambda} \cdot \frac{1}{\sqrt{n}} \frac{\rho_{eq}}{2W} \]

where \( v_{s0} \) is the stack’s equivalent sound velocity associated with the S0 lateral mode, \( \lambda \) is the acoustic wavelength, \( E_{eq} \) and \( \rho_{eq} \) are the equivalent modulus of elasticity and the density respectively, and \( W \) is the electrode pitch.

The equivalent density and elastic modulus are weighted values by the thicknesses:

\[ \rho_{eq} = \frac{\sum \rho_i t_i}{\sum t_i} \quad E_{eq} = \frac{\sum E_i t_i}{\sum t_i} \]

where \( n \) is the number of different layers, and \( t_i \) is the thickness of the \( i \)-th layer. Given the thickness ratios between piezoelectric and metals, the resonance frequency is mostly set by \( W \). Unlike BAW devices [27], \( f_r \) is therefore decoupled from the piezoelectric layer thickness, allowing fabrication of devices operating at different frequency on the same wafer.

The fabrication, schematically displayed in Fig. 1, starts with the patterning of the bottom Pt metal plate through lift-off onto high resistive silicon wafers (>10k ohm-cm). Then, the piezoelectric layer is deposited via DC Magnetron sputtering using an Al0.83Sc0.17 target. The top metal (Pt) is deposited and later patterned in interdigitated (IDT) electrodes via dry etching. In order to define the resonator shape in the AlScN, we first deposit a 1.5 μm thick SiO2 hard mask, and we pattern it later in the interdigitated (IDT) electrodes via dry etching. In order to define the resonator shape in the AlScN, we first deposit a 1.5 μm thick SiO2 hard mask, and we pattern it later in the interdigitated (IDT) electrodes via dry etching. In order to define the resonator shape in the AlScN, we first deposit a 1.5 μm thick SiO2 hard mask, and we pattern it later in the interdigitated (IDT) electrodes via dry etching.

To extract Q, the admittance response of a device, subtracted of the off-resonance background, is fitted to a Lorentzian curve. This method is equivalent to extracting Q using -3dB points in case of clean response. However, when spurious modes are present, especially in close proximity of the resonance, the Lorentzian fit is less affected and thus a better choice [30]. The electromechanical coupling is computed as the ratio of the motional capacitance (C_m) and the static capacitance of the device (C_0) as in (3):

\[ k_i^2 = \frac{\pi^2}{8} \frac{C_m}{C_0} \]
swept from 0.25 \( \lambda \) to 0.9 \( \lambda \) in steps of 0.5 \( \lambda \). This fine step is chosen to detect potential sharp transition in \( Q \). Regarding B, three dimensions are used: 0.15 \( \lambda \), 0.2 \( \lambda \), and 0.25 \( \lambda \). The anchor length (\( L_a \)) is fixed to \( \lambda \).

Fig. 4(b) shows unloaded \( Q \) as function of \( W_a \) for the three bus configurations in different colors. Each data point is the average of 3 identical devices.

The three bus configuration show similar trend. In particular, the maximum \( Q \) is always measured at \( W_a=0.45 \lambda \). The peak is followed by a local minimum and subsequently, at \( W_a=0.55 \lambda \), about 80\% of the maximum \( Q \) is recovered. In contrast, the bus dimension does not change the trend but modulates the \( Q \) amplitude, having the highest average \( Q \) when the bus length is \( \lambda/4 \) [13].

Even though the values of \( Q \) are lower than what obtained in AlN, we observe that higher \( Q \) are measured in devices at higher frequencies (Fig. 5(b)). In particular, the highest \( Q \) is measured for a device resonating at 388 MHz (Fig. 5(a)) and is in excess of 1600. We believe that a dependency of \( Q \) in the resonator length (\( L \)) could explain the \( Q \) enhancement as the pitch is decreased. As a matter of fact, \( L \) is kept constant to 140 \( \mu \)m for all the CMRs, which implies \( L=3.5 \lambda \) for a CMR working at 198 MHz and \( L=7 \lambda \) for a CMR operating at 388 MHz. Finally, the \( Q \) sensitivity to \( W_a \) computed as \((Q_{\text{max}} - Q_{\text{min}})/(Q_{\text{max}} + Q_{\text{min}})\) on devices with identical \( L \) is 72\%, 68\%, and 39\% for devices operating at 151 MHz, 194 MHz, and 388 MHz respectively. This suggests that at higher frequencies the relative contribution of anchor dissipation is smaller. This is likely to be linked to the fact that the ratio \( L/\lambda \) drops.

### B. Electromechanical coupling

We also measure the electromechanical coupling of all devices, for different pitches. In the case of \( \lambda = 40 \mu \)m, the average \( k_t^2 \) of all the 126 measured devices is 4.42\%, representing a 2.2\times improvement with respect to identical CMRs fabricated in AlN (\( k_t^2 \approx 2\% \)). As an example, Fig. 4(a) shows the admittance response of a resonator operating at 194 MHz with the relative mBVD fit and parameters extraction.

After characterizing devices with different resonance frequencies (6 devices with highest \( Q \) for each frequency), we show that the average \( k_t^2 \) decreases as the frequency increases, reaching a minimum of 3.37\% for the set of devices at ~490 MHz (Fig. 5(b)). After comparing our experimental results to FE simulations that fringing effect between adjacent electrodes happens and degrades \( k_t^2 \) for narrower pitches. This effect is more pronounced for AlScN than for AlN since the acoustic velocity of the former is smaller than the latter. However, the fringing effect does not seem to be the dominant factor, but rather a secondary player compared to the appearance of spurious modes. Importantly, our findings point towards a degradation of \( k_t^2 \) due mainly to spurious modes, rather than a degradation due to material properties, i.e. the piezoelectric coefficient of our AlScN is frequency independent.

### C. Material parameter extraction

The starting point to extract the material parameters is to fit to (1) the resonant frequencies, as function of the pitch, of the ensemble of the fabricated CMRs, which in our case operate at 4 different frequencies (Fig. 6(b)). The devices have \( W=26 \mu \)m, \( W=20, W=10, \) and \( W=8 \mu \)m (Fig. 2 and Fig. 3) and they have 3, 3, 5, and 7 fingers respectively in order to maintain similar resonator width and thus, simple simultaneous release. It is assumed that the density of AlScN is 3255 kg/m\(^3 \) [23], and the equivalent density (\( \rho_{eq} \)) is given as an input parameter to a least square algorithm to extract the equivalent modulus of elasticity (\( E_{eq} \)). Density and the Young modulus for Pt are 21450 kg/m\(^3 \) and 168 GPa, respectively.

As seen in (2), the thicknesses of the layers have to be known in order to properly compute the equivalents for the stack. For this reason, a cross section of the fabricated wafer is analyzed using scanning electron microscope (SEM). In Fig. 6(a), it can be seen that the bottom and top metal layers are about 100 nm thick while the piezoelectric layer is about 1.2 \( \mu \)m thick. After obtaining \( E_{eq} \), (2) is reversed to compute \( E_{AlScN} \) as below:

\[
E_{AlScN} = \frac{E_{eq} T_{tot} E_{Pt} T_{Pt}}{T_{AlScN}} \tag{4}
\]

In CMRs, the equivalent elasticity modulus can be assumed to be equal to \( C_{11} \), the stiffness component involved in the lateral expansion. The obtained \( E_{eq} = C_{11} = 339.8 \) GPa closely matches the ab-initio calculations reported in literature for AlScN [32], confirming a softening (lower acoustic velocity) of the piezoelectric material with respect to AlN (\( \approx 410 \) GPa). As an example to illustrate this difference, a device with \( W=20 \mu \)m, with the same thicknesses composing the stack, gives a resonance frequency of 194 MHz for AlScN and 219 MHz for AlN.

Devices with \( W=20 \mu \)m (3 fingers) with slightly different \( L \) are used to extract the relative permittivity of AlScN. Equation (5) is used to fit the measured static capacitance \( C_0 \) as function of resonator active length (\( L_{active} = L - 2B \)). The bus is an inactive area because the bottom metal is removed by design underneath it. The relative permittivity is then computed as:

\[
\varepsilon_{r33} = \frac{3}{2} \cdot C_0 \cdot \frac{T_{pze}}{W_e L_{active}} \tag{5}
\]
where $T_{\text{piez}}$, $W_{e}$, $L_{\text{active}}$ are the piezoelectric thickness, the electrode coverage, and the active length of the resonator (Fig. (7)). As it is expected, $C_0$ has an increasing trend as the resonator is longer. The extracted $\varepsilon_{33}$ is 12.93 at 194 MHz. This value is in line with what previously reported for FBAR [23]. The small difference in $\varepsilon_{r33}$ can be explained by the fact that in a CMR in LFE configuration, unlike for FBAR, the E lines are not entirely vertically distributed. Also, by comparing the measured and the numerically simulated (FEM) $C_0$ values we verified that $\varepsilon_{r33}$ can be assumed constant in this frequency range.

The electromechanical coupling $k_t^2$ can be expressed as follows:

$$K^2 \approx \frac{d_{31}^2}{\varepsilon_{11}^F \varepsilon_{33}^F} = \frac{d_{31}^2}{\varepsilon_0 \varepsilon_{r33}^F E_{eq}} \quad (6)$$

where Eq. (6) is valid since the electrode’s thickness is <1/10 of the piezoelectric layer’s thickness.

If Eq. (6) is reversed, now that $E_{eq}$ and $\varepsilon_{r33}$ are known and, given that the average $k_t^2$ is 4.42 % (at 194 MHz) one can compute the piezoelectric ($d_{31}$) coefficient for Al$_{0.83}$Sc$_{0.17}$N. The extracted $d_{31}$, at 194 MHz, is -3.89 pm/V, which represents a 2.25$\times$ improvement with respect to AlN ($d_{31, \text{AlN}} = -1.73$ pm/V). This extracted value is validated by excellent matching with ab-initio calculated value for $d_{31}$ (-3.87 pm/V) [33].

**D. Temperature compensation**

MEMS-based oscillators enable low phase noise, low energy consumption and single-chip oscillator solutions [34, 35]. Among different technologies, AlN based MEMS resonators have larger power handling than Si based resonators and a greater $k_t^2$, which enables wider tuning range [36]. On the other hand, in AlN based MEMS there is no zero TCF orientation unlike in crystalline materials like quartz or Silicon [37]. The typical approach for TCF compensation in some MEMS relies on the use of SiO$_2$ thin layers attached to the resonator stack [38, 39]. Since SiO$_2$ has the rare characteristic of a positive first-order temperature coefficient of elasticity (TCE) [40], it can be used to compensate the negative TCF of the rest of the stack. In fact, people have used AlN-based resonators to demonstrate temperature sensors that operate linearly at different temperatures, depending on the amount of compensation [41].

In all of previous works, thermal oxide is used and it is often placed below the bottom metal. That is, the desired SiO$_2$ thickness is analytically estimated a priori. Thus, a very fine analytical model and control of every thickness involved in the process is required.

Instead, we take a more flexible approach to easily obtain zero-TCF, using SiO$_2$ compensation layer, in already fabricated devices: we sputter SiO$_2$ on top of released resonators, using a stencil mask. The SiO$_2$ thickness is checked with a mechanical profilometer in a region outside the resonator. This method allows simultaneous compensation of multiple frequencies and, at the same time, it does not require any a priori estimation of the needed thickness. As a consequence, after characterization of the TCF in a limited number of devices, the SiO$_2$ thickness can be further adjusted without the need of fabricating a new wafer. The three sets of devices resonating at 194 MHz (W=20 μm), 388 MHz (W=10 μm), and 479 MHz (W=8 μm) are characterized. Measurements are taken on a heated chuck, starting at 25°C up to 145°C with a sampling step of 30°C.

In Fig. 8(a) the relative frequency variation as function of temperature is shown for devices operating at 194 MHz. The reference CMRs without oxide has a linear decreasing trend with a slope of -27.6 ppm/°C. By adding SiO$_2$, the negative trend is mitigated. 1.5 μm of SiO$_2$ reduces the 1$^{\text{st}}$ order TCF by a factor of 9. By adding thicker SiO$_2$, a nearly zero TCF can be obtained. However, when the SiO$_2$ thickness is larger than the resonator stack, the response in temperature becomes quadratic (i.e. relative frequency variation when 2.25 μm of SiO$_2$ is added). Table II report the 1$^{\text{st}}$ and 2$^{\text{nd}}$ order TCF as function of the SiO$_2$ thickness for the three different frequencies. One can estimate the optimal SiO$_2$ thickness looking at the 1$^{\text{st}}$ order TCF, which is displayed in Fig. 8(b) for the three sets of devices. A linear fit is used to estimate the optimal SiO$_2$ thickness to obtain a zero 1$^{\text{st}}$ order TCF. CMRs operating at different frequencies require slightly different SiO$_2$ thickness but always around 1.5 μm. For this thickness, the 2$^{\text{nd}}$ order TCF is neglected since the quadratic term is negligible.

When targeting both a particular frequency and temperature compensation, one also needs to consider that adding SiO$_2$, a softer material in the stack, causes a downshift of the resonant frequency. As it is seen in Eq. 1, the equivalent sound velocity depends on the thicknesses of all materials in the stack. In this study, the sputtered SiO$_2$ leads to a 9% and 12% drop of the frequency when 1.5 μm and 2.25 μm of SiO$_2$ are added respectively (Fig. 8(c)). Moreover, even though a full study of Q and $k_t^2$ dependency on SiO$_2$ thickness is not conducted here, it is expected that the thicker the layer, the more degradation will be observed.

**IV CONCLUSIONS**

In this paper we demonstrate the fabrication of Al$_{0.83}$Sc$_{0.17}$N CMRs. Our results show an improvement in the electromechanical coupling of more than 2$\times$ with respect to identical resonators in pure AlN, at around 200 MHz. A drop in $k_t^2$ is observed at higher frequencies mainly due to the presence of spurious resonances. The highest $Q$, in excess of 1600, is obtained for a CMR operating at 388 MHz. Geometrical optimization, especially in the resonator length (i.e. scaling the resonator length according to $\lambda$), could improve Q in CMRs operating at lower frequencies. Moreover, as AlScN material parameters are extracted, modelling will open to a better understanding of the dissipation mechanisms for this new piezoelectric material.

From the electrical measurements several material properties are extracted. The extracted $C_{11}$=339.8 GPa for Al$_{0.83}$Sc$_{0.17}$N closely matches the ab-initio calculation present in literature [32]. Similarly, the relative permittivity is close to what has been reported for BAW [23]. Subsequently, the $d_{31}$ piezoelectric coefficient is computed. The extracted $d_{31}$ value of -3.89 pm/V matches the ab-initio prediction [33] and for devices operating around 200 MHz, corresponds to a 2.25$\times$ enhancement with respect to pure AlN. Finally, we report the experimental result of passive compensation of the frequency.
temperature drift using sputtered SiO₂ on top of the CMRs. Differently from previous studies, in this work the SiO₂ layer is added on top of already released resonators. This results in an unnecessary a priori accurate estimation of the compensation layer thickness and enables the measurement of the same resonator with different oxide thicknesses. We show that a SiO₂ thickness around 1.5 μm allows near zero TCF for devices operating up to 500 MHz, with a reasonable fabrication processing.

ACKNOWLEDGEMENTS

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REFERENCES


Figure 1: Process flow used in this work for the fabrication of AlScN 1-port CMRs: (a) lift-off of the bottom Ti+Pt on HR (>10000 ohm·cm) Si wafer. (b) Dry etching of the top Pt for IDT patterning. (c) Resonator shaping via Cl- chemistry and using a SiO2 hard mask. (d) Resonator release through SF6.

Table I: AlScN etching recipes and relative etching rates.

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Figure 2: SEM pictures of three CMRs operating at different frequencies, obtained by lithographic tuning of W: 26 μm (a), 10 μm (b), and 8 μm (c), which correspond to a resonant frequency of 150 MHz, 388 MHz, and 479 MHz respectively. In Fig. (a) all the designed parameters are displayed.
Figure 3: (a) SEM image of a 194 MHz CMR (W=20 μm); the inset (in yellow) is a zoom-in of the resonator edge to show steep sidewall angles. (b) Top view of a zoom-in of Fig. (a) (red dashed line) shows the sidewall angle obtained through optimized Cl-chemistry etching recipe and using a SiO2 hard mask. The estimated sidewall angle is 70 degrees.

Figure 4: (a) Admittance response of a 1-port CMR resonating at 193 MHz with bus = 0.15 λ, Wa = 0.45 λ, La = λ, and 3.5 λ long. The normalized root mean square error (NRMSE) of the fit is 0.89, ensuring excellent parameter extraction. Fit using the mBVD model (blue) is overlaid to measured admittance curve (red). (b) Unloaded Q as function of Wa for resonators 3.5λ long and with fixed La = λ. Each point is the average response of 3 identical devices. Three configurations are showed with bus 0.15 λ long (green triangles), 0.2 λ long (blue diamonds), and 0.25 λ long (black circles). In the three different configurations it is evident the presence of two peaks and one deep for Wa = 0.5λ. Maximum Q is always found at Wa = 0.45 λ and a second local maxima is found at Wa = 0.55 λ with about 20% lower Q. The average electromechanical coupling is 4.42%. 

\[ Q_{un} = 783 \]
\[ \mu = 621 \]
\[ f_p = 193.31 \text{ MHz} \]
\[ f_s = 196.72 \text{ MHz} \]
\[ k_e^2 = 4.58 \% \]
Figure 5: (a) Admittance response of a 1-port CMR resonating at 388 MHz with bus = 0.15 λ, Wa = 0.4 λ, La = λ, and 3.5 λ long. The NRMSE of the fit is 0.71, ensuring excellent parameter extraction regardless of spurious resonances present in the admittance response. Fit using the mBVD model (blue) is overlaid to measured admittance curve (red). (b) Average $k_1^2$ of 6 devices showing highest $Q_m$ for each resonant frequency (black dots) and measured maximum $Q_m$ (red triangles). The electromechanical coupling has a decreasing trend as the frequency increases because of more severe spurious at higher frequencies. On the other hand, the highest $Q_m$ is measured for a device resonating at 388 MHz.

Figure 6: (a) Cross section of the fabricated wafer for assessment of the layers’ thicknesses. The thickness of the top and the bottom metal is 100 nm, while the piezoelectric layer thickness is 1.2 μm. (b) Measured resonant frequencies as a function of the pitches (black diamonds). Data are fitted, using a nonlinear square fitting algorithm to (1) to extract the equivalent modulus of elasticity of the whole stack.
Figure 7: (a) Measured static capacitance as function of the resonator length (black dots). Each point is the average of 56 devices with identical resonator length. The data are fitted (blue dash line), using a nonlinear square fitting algorithm, to the equation of $C_0$ (in the inset) to extract the relative dielectric permittivity of AlScN. Above the graph, a schematic of the capacitive behavior of the resonator is displayed. As expected from the equation for $C_0$ showed in the inset, longer resonators correspond to higher measured static capacitance.

Figure 8: (a) Relative frequency variation as a function of the substrate temperature. Each point is the average of 3 CMRs resonating at 194 MHz. In different colors are reported the measured relative frequency variations for different thickness of SiO$_2$ deposited on the resonators: the reference with no oxide (black dots), 1.25 μm of SiO$_2$ (blue squares), 1.5 μm (green diamonds), and 2.25 μm (red triangles). It can be noted that AlScN has intrinsically a linear negative variation in frequency as temperature increases of -27.6 ppm/°C. By adding SiO$_2$ to the resonating stack, it is possible to reduce the negative slope, even though when the SiO$_2$ thickness outweigh the stack thickness the linear trend is replaced by a quadratic response in temperature. (b) 1st order TCF up to 145 °C. A zero TCF is obtained for different SiO$_2$ thicknesses depending on the operating frequency of the resonator. Points are the experimentally extracted TCF, the lines are a linear interpolation to predict the zero TCF SiO$_2$ thickness. In particular, a zero 1st order TCF is predicted at 1.65 μm of SiO$_2$ for devices resonating at 194 MHz and for slightly thinner SiO$_2$ thickness for devices resonating at 388 MHz and 479 MHz. (c) Admittance curve of a CMR operating at 194 MHz without SiO$_2$ (black), with 1.5 μm of SiO$_2$ (blue), and 2.25 μm (green). The addition of SiO$_2$ leads to a drop of 9% and of 12% in the resonant frequency for 1.5 μm and 2.25 μm of SiO$_2$, respectively.
Table II: 1st and 2nd order TCF for devices resonating at 194 MHz, 388 MHz, and 479 MHz in function of SiO$_2$ thicknesses.

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