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Influence of Carbon Incorporation on the Microstructure, Morphology, Mechanical Properties, Tribological Behavior and Corrosion Resistance of TiAlCN Coatings Deposited Via Reactive HiPIMS

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This study explores the synthesis and characterization of Titanium Aluminum Carbon Nitride (TiAlCN) coatings, a pioneering advancement in surface engineering. Using reactive High Power Impulse Magnetron Sputtering (HiPIMS), we deposited TiAlCN coatings with varying carbon content (1.3 - 58.1 at.%) by modulating the acetylene flow rate. X-ray diffraction analysis revealed a carbon solubility limit of 17 at.% in the TiAlN structure, beyond which TiAl(CN) nanocrystals and an amorphous carbon phase emerged. This structural evolution significantly impacted the coatings' properties. Notably, increasing carbon content noticeably reduced the coefficient of friction from 0.62 (TiAlN) to 0.22 (42 at.% C), enhancing tribological performance. However, high carbon concentrations impeded aluminum diffusion, hindering the formation of a protective Al_2O_3 layer and consequently diminishing corrosion resistance. Additionally, the presence of amorphous carbon between grains at elevated carbon levels led to a reduction in the coatings' mechanical properties.

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Influence of carbon incorporation on the microstructure, morphology, hardness, Young modulus of TiAlCN coatings deposited via reactive-HiPIMS

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Presentation outlines

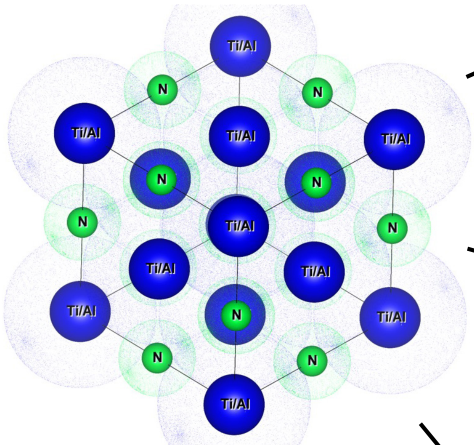
I- Introduction

Why is TiAlN coating?

Coating	Microhardness, $HV_{0.05}$	Maximum service temperature, °C	Coefficient of friction against steel (dry)	Color
TiN	2300	600	0.4	Gold-yellow
AlCrN	3200	1100	0.35	Bright grey
TiCN	3000	400	0.4	Blue grey
WC/C	1500	300	0.2	Anthracite
CrN	1750	700	0.5	Silver grey
DLC	2000	350	0.2	Black
TiAlN	3300	900	0.35	Violet grey
TiCrN	2100	700	0.5	Dark grey

Tabrizi et al. Journal of Surface Investigation: X-ray, Synchrotron and Neutron Techniques, 15(6), 1217-1224.

I- Introduction



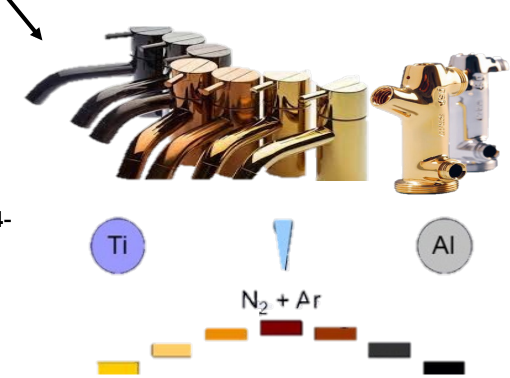
TiAlN structure

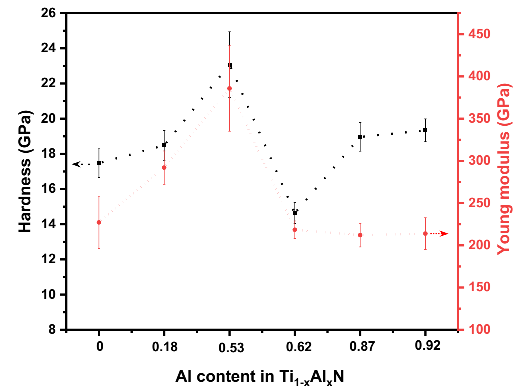
M. Lahouij et al. J. Mater. Eng. Perform. (2024). https://doi.org/10.1007/s11665-024-09640-y.

Mechanical & industrial parts

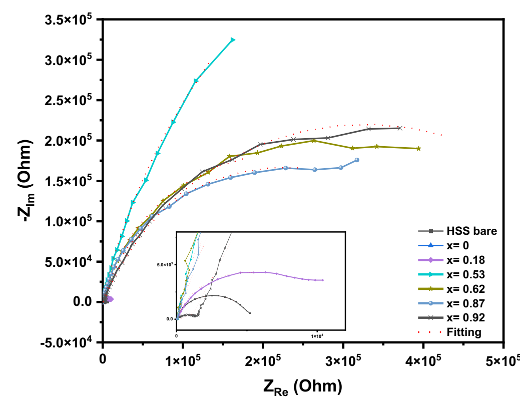
Medical implants

Thermal & decorative coatings



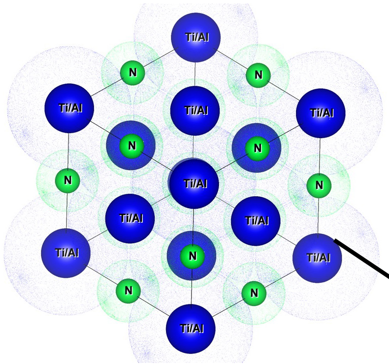


- Improved mechanical, tribological and corrosion properties as a function of the Al content in the coatings

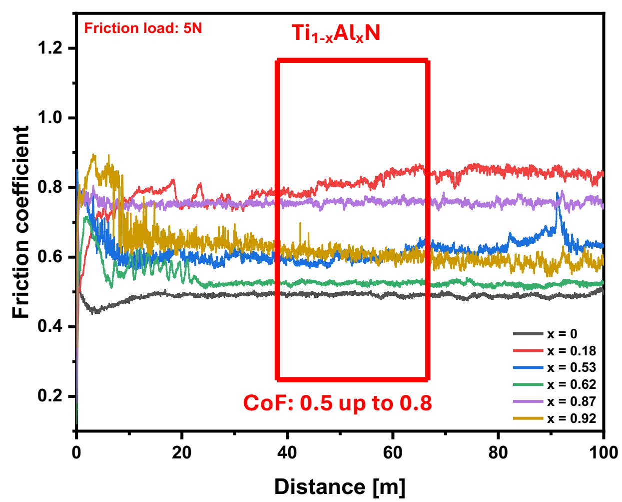


I- Introduction

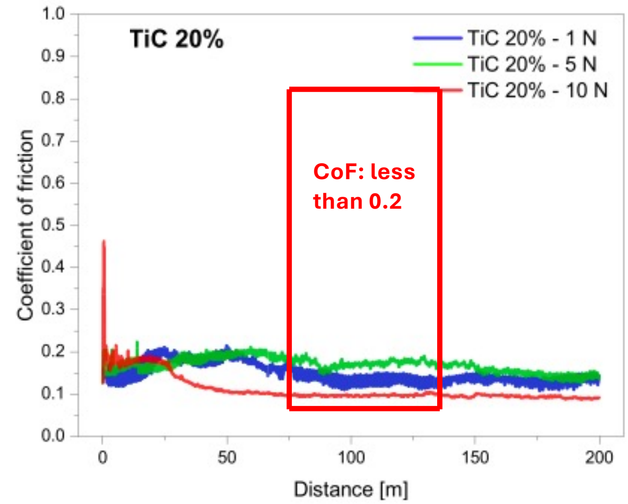
Motivation for a low friction coefficient material



M. Lahouij et al. J. Mater. Eng. Perform. (2024). https://doi.org/10.1007/s11665-024-09640-y.



H. Larhlimi, et al. Int. J. Refract. Met. Hard Mater. 120 (2024) 1–10. https://doi.org/10.1016/j.ijrmhm.2024.106599.



What about TiAlCN??

II- Deposition and Characterization of TiAlCN Coatings

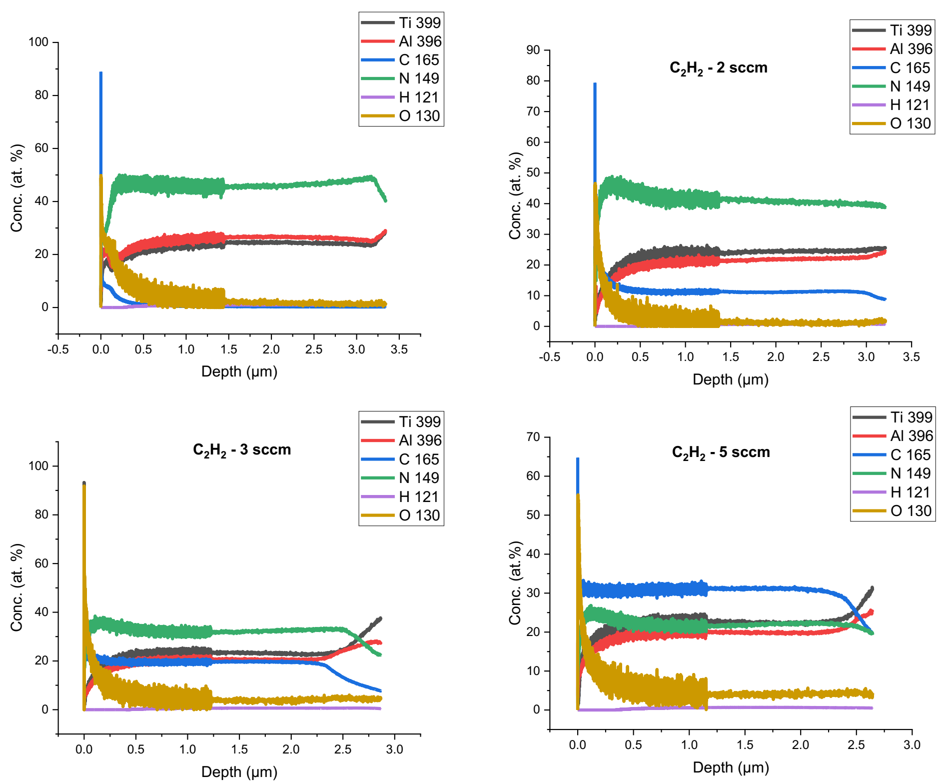
II-1. Experimental procedure

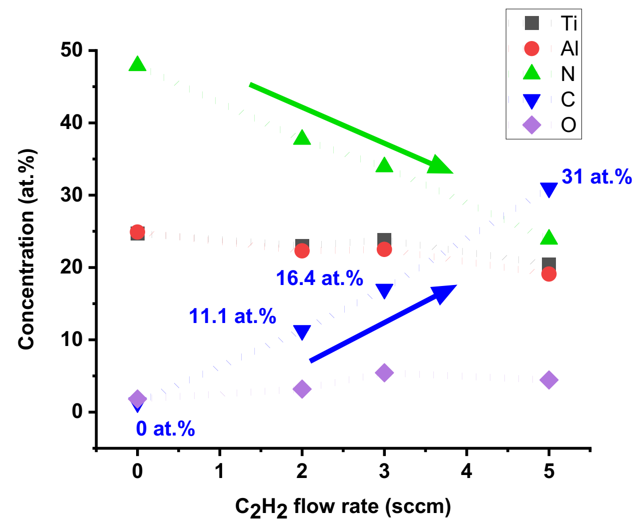
Gas Pressure	Uncontrolled pressure
Average Power	5 kW (HiPIMS)
Gas mixture	Ar (100 sccm) + N_2 (10 sccm) + C_2H_2 (0 to 5 sccm)
Substrate	Si & Carbon steel
Etching	25 min (- 700 V)
Interlayer	Ti-Al (≈ 500 nm)
Bias Voltage	- 80 V
Deposition temperature	No substrate heating

II- Deposition and Characterization of TiAlCN Coatings

II-2. Elemental composition

Glow Discharge Optical Emission Spectroscopy (GDOES)

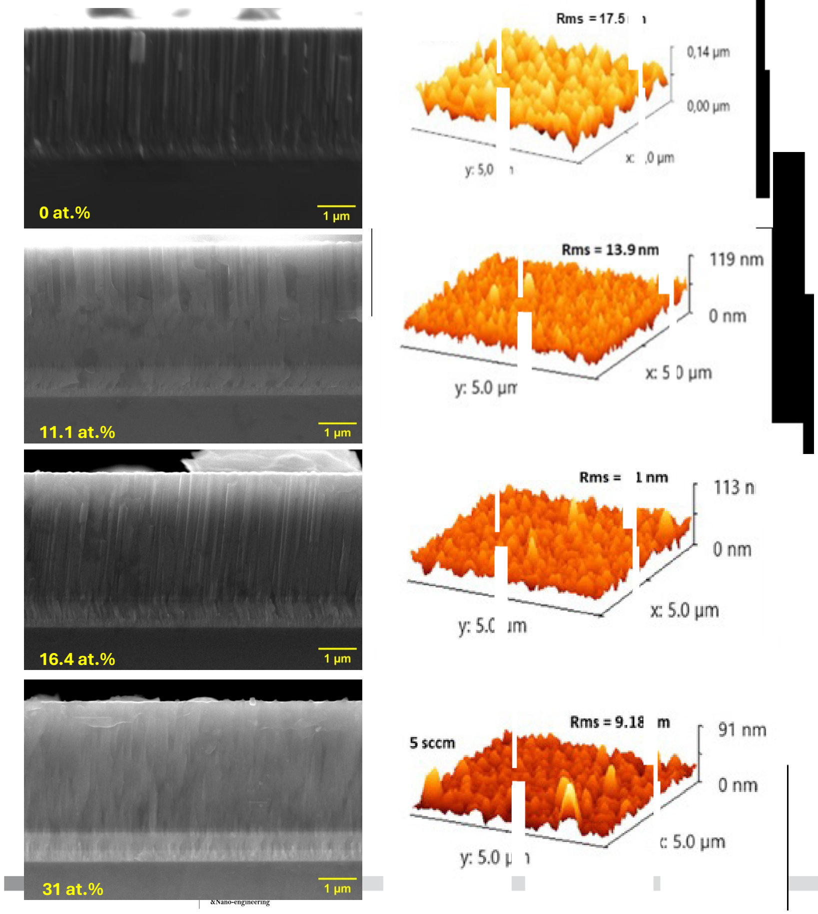




- The carbon concentration increases over the decrease of Nitrogen concentration.
- A decrease in the metal elements was also observed

II- Deposition and Characterization of TiAlCN Coatings

II-2. Morphology and Roughness

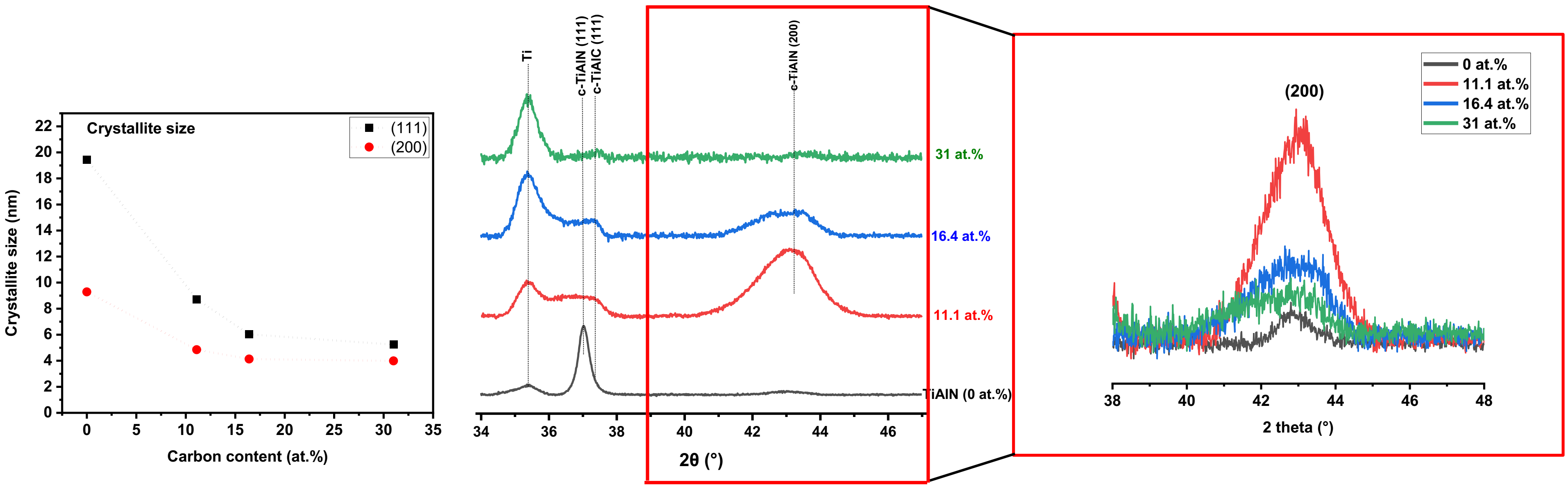


- SEM images show a dense microstructure with a morphology alternating from continuous to glassy features with high carbon concentration coatings.

- AFM illustrates a reduction of the coating's roughness as the carbon increases in the coating.

II- Deposition and Characterization of TiAlCN Coatings

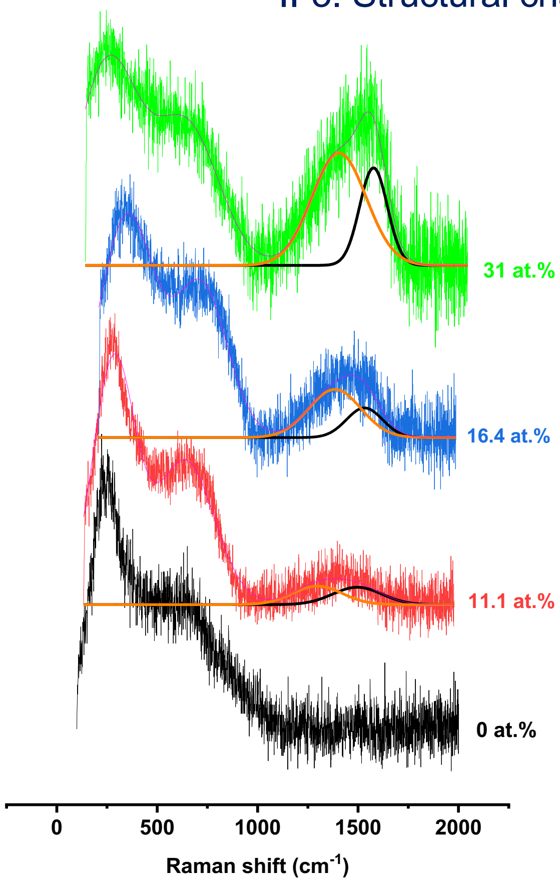
II-3. Structural characterization (XRD)



- TiAlN crystallize in a NaCl-structure type with a preferred orientation of (111)
- An amount of 11.1 at.% of C leads to refine the c-TiAlCN microstructure with a preferred orientation of (200)
- As the Carbon content increase the signal from the interlayer is increased ===> amorphization of the microstructure

II- Deposition and Characterization of TiAlCN Coatings

II-3. Structural characterization (Raman)



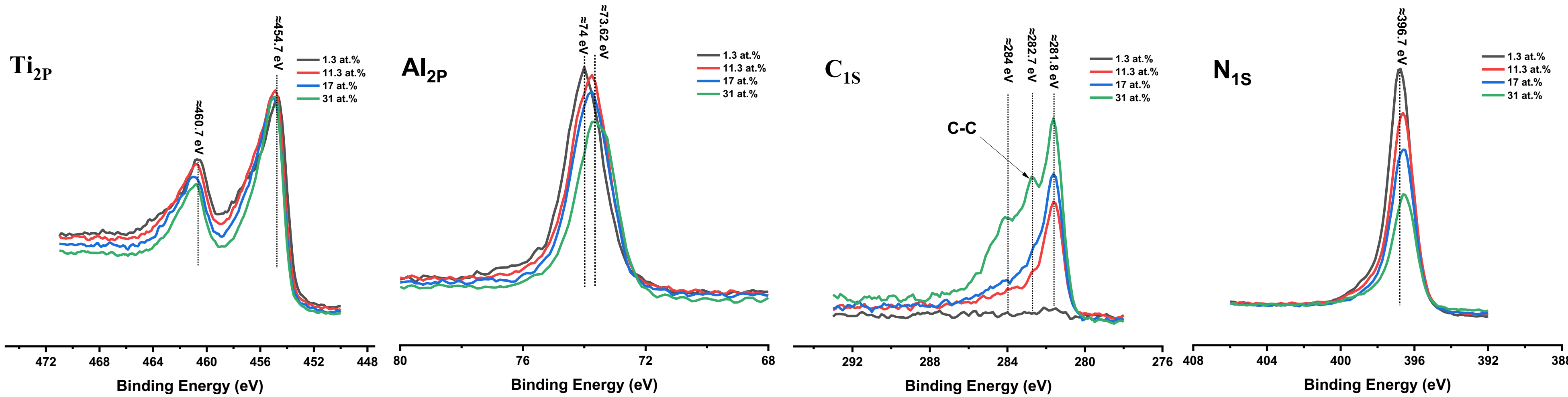
Samples	D peak			G peak		
	Peak position (cm^{-1})	FWHM	I_D	Peak position (cm^{-1})	FWHM	I_G
TiAlN (0 at.%)	___	___	___	___	___	___
11.1 at.%	1349.9	360.0	0.06	1529.8	200.16	0.04
16.4 at.%	1356.6	336.5	0.18	1532.2	164.55	0.07
31 at.%	1364.8	330.2	0.33	1534.4	158.42	0.28

- A small amount of the a-C is detected within the coating at 11.1 at.% of C
- The **peak wave numbers** shifted toward **higher values**
- A **decrease** in the **FWHM** of the D and G bands

Increased sp^2 graphitic ordering

II- Deposition and Characterization of TiAlCN Coatings

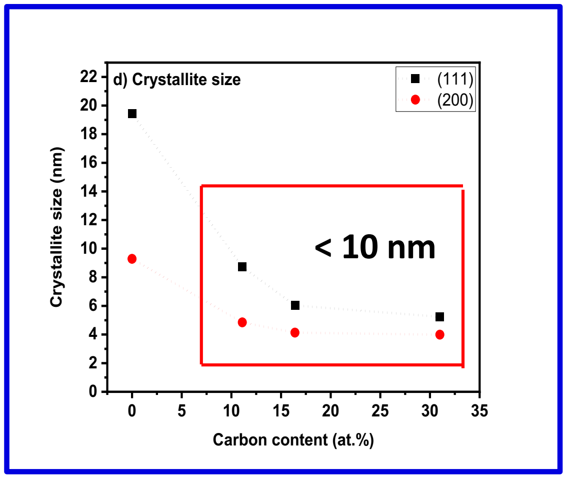
II-3. Structural characterization (XPS)

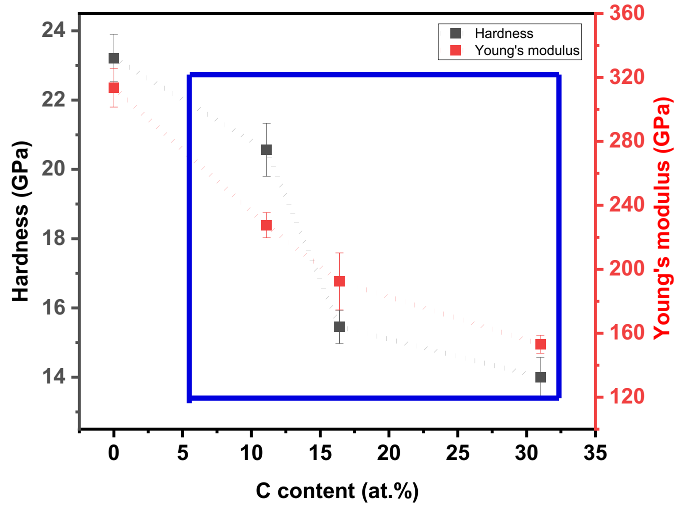


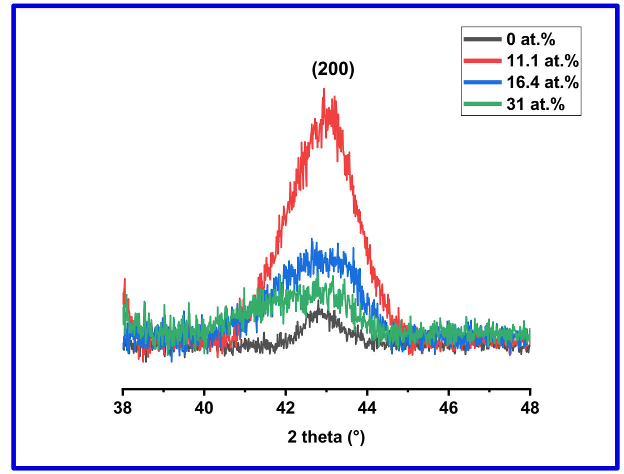
- Substitution of N atoms with those of C.
- A low binding energy (≈73.37 eV), attributed to the formation of the Al-C phase.
- TiAl(CN) solid solution phase in the form of a nanocrystalline (Ti, Al)C grains trapped in an amorphous carbon matrix.

III- Mechanical & Tribological properties

III-1. Mechanical properties



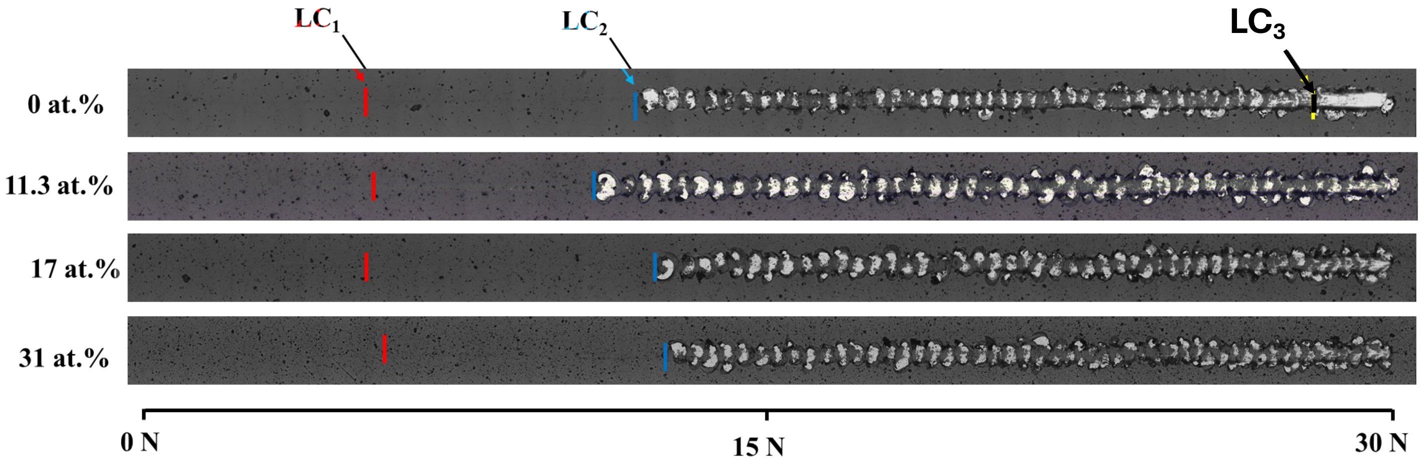




❖ A decrease in the Nano-hardness and the Young modulus of TiAlCN as the carbon content increases. This behavior can be attributed to the **change in the crystalline preferred orientation** from (111) to (200), **The increase in the a-C phase** and the **reduction in the crystallite size** (with an order less than 10 nm ===> The inverse of the Petch-Hall effect)

III- Mechanical & Tribological properties

III-2. Coatings adhesion



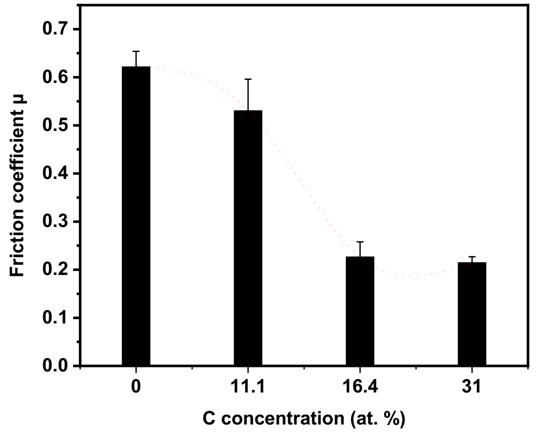
sample	H/E	H^3/E^2 (GPa)
0 at.%	0.07	0.13
11.1 at.%	0.09	0.16
16.4 at.%	0.09	0.13
31 at.%	0.09	0.13

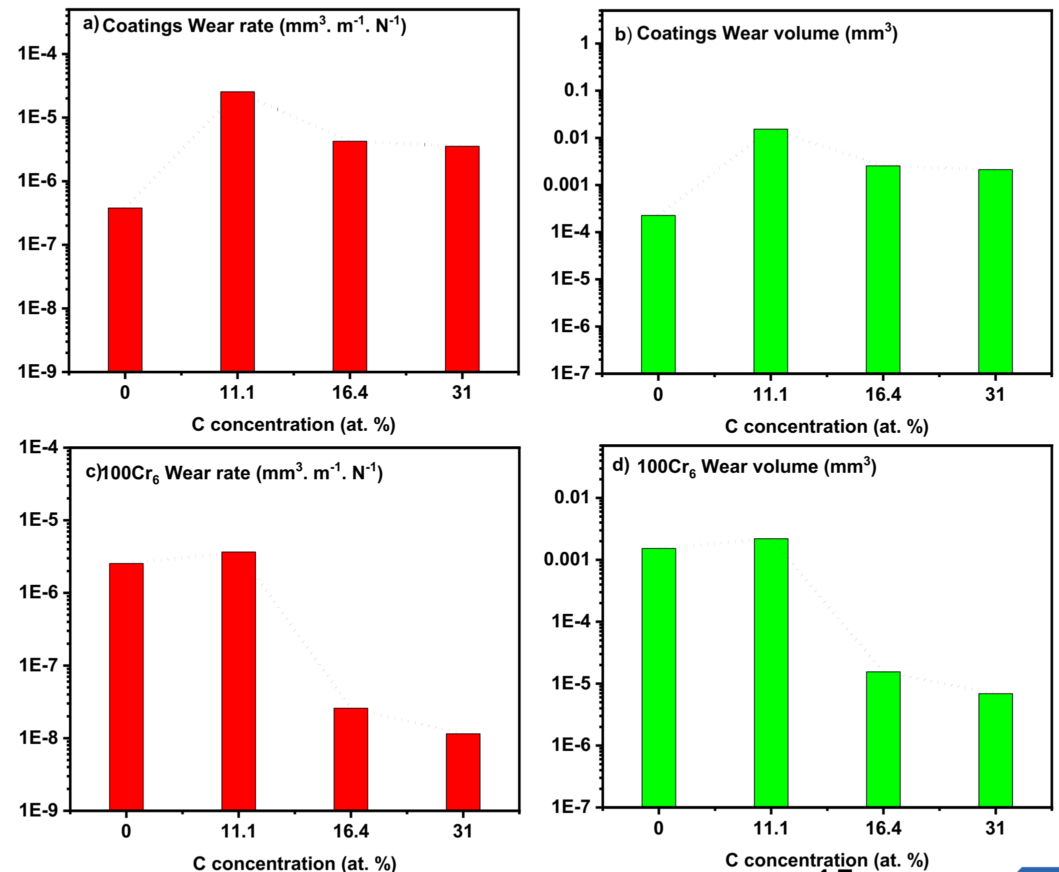
Samples	First crack appearance	Spallation	Total delamination
	LC_1 (N)	LC_2 (N)	LC_3 (N)
0 at.%	5.5	11.92	28.47
11.1 at.%	5.77	10.91	> 30
16.4 at.%	5.56	12.31	> 30
31 at.%	6.03	12.68	> 30

- Overall, adhesion performance remained strong, with LC_3 values exceeding 30 N for all samples;
- Improved LC_3 in C coatings correlated to their high elastic strain parameter (H/E)

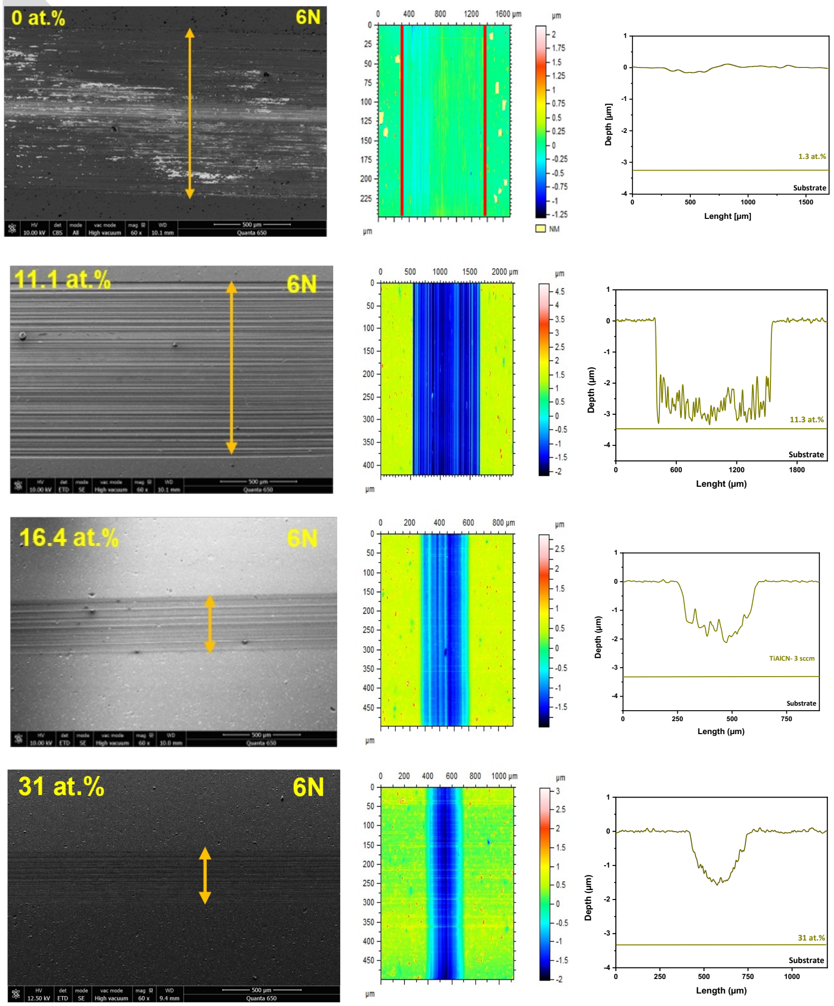
III- Mechanical & Tribological properties

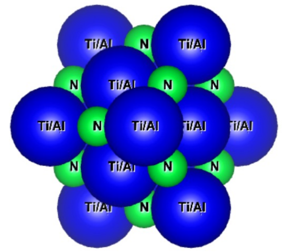
III-2. Tribological properties (Sliding experiments against 100Cr6 steel balls for 100 m and under a load of 6N)





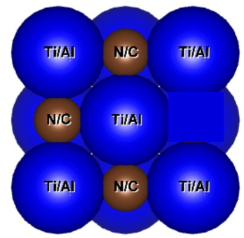
- The friction coefficient is reduced from 0.62 to 0.199: Graphitization of the a-C.
- The wear rate shows inconsistent trends:
  - Increases for the coatings with 11.3 at.%
  - Decreases for the coatings at higher carbon content.





(111) Preferred orientation

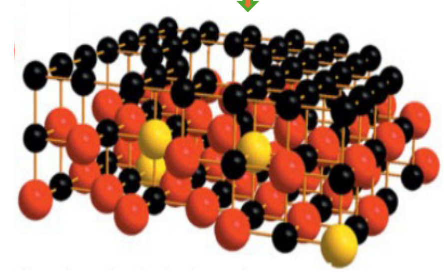
Hard and compact structure



(200) Preferred orientation

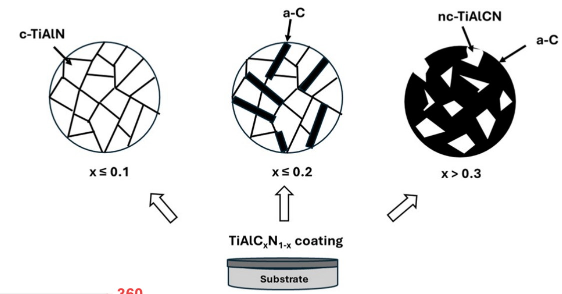
Lesser hard, the structure contains vacancy defects,

Sliding experiments

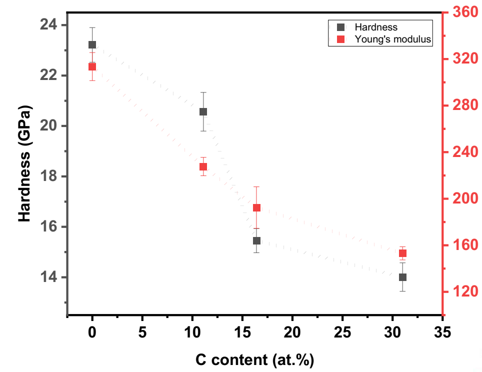


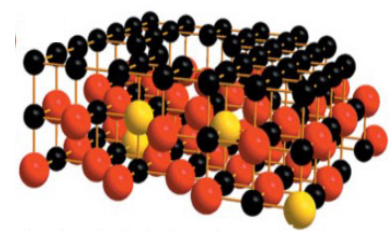
Segregation of the C atoms to the surface due to the weaker bond Al-C

IV- Conclusions & Perspectives



- ❑ A transition from c-TiAlN (111), c-TiAlCN (200) to nanocomposite microstructure is observed as the C at.% ↑
- ❑ The nano-hardness and Young's modulus of the coating show a reduction as the carbon content increases
- ❑ The CoF of the deposited coatings shows a reduction by more than 50% (from 0.7 to 0.2)
- ❑ The wear rates of the coatings shows a slight increase mainly attributed to the segregation of the carbon atoms from the TiAlCN structure.





- ➢ What could be the influence of carbon incorporation on the thermal resistance?
- ➢ Reduce the Al content to study its effect on the mechanical and wear resistance.
- ➢ Investigate the sputtering of TiAlCN coatings using a carbon target.

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