Properties of amorphous SiC films

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Istituto Nazionale di Fisica Nucleare LNL Laboratori Nazionali di Legnaro

Thin Film Optics Group GOLD Grupo de Óptica de Láminas Delgadas

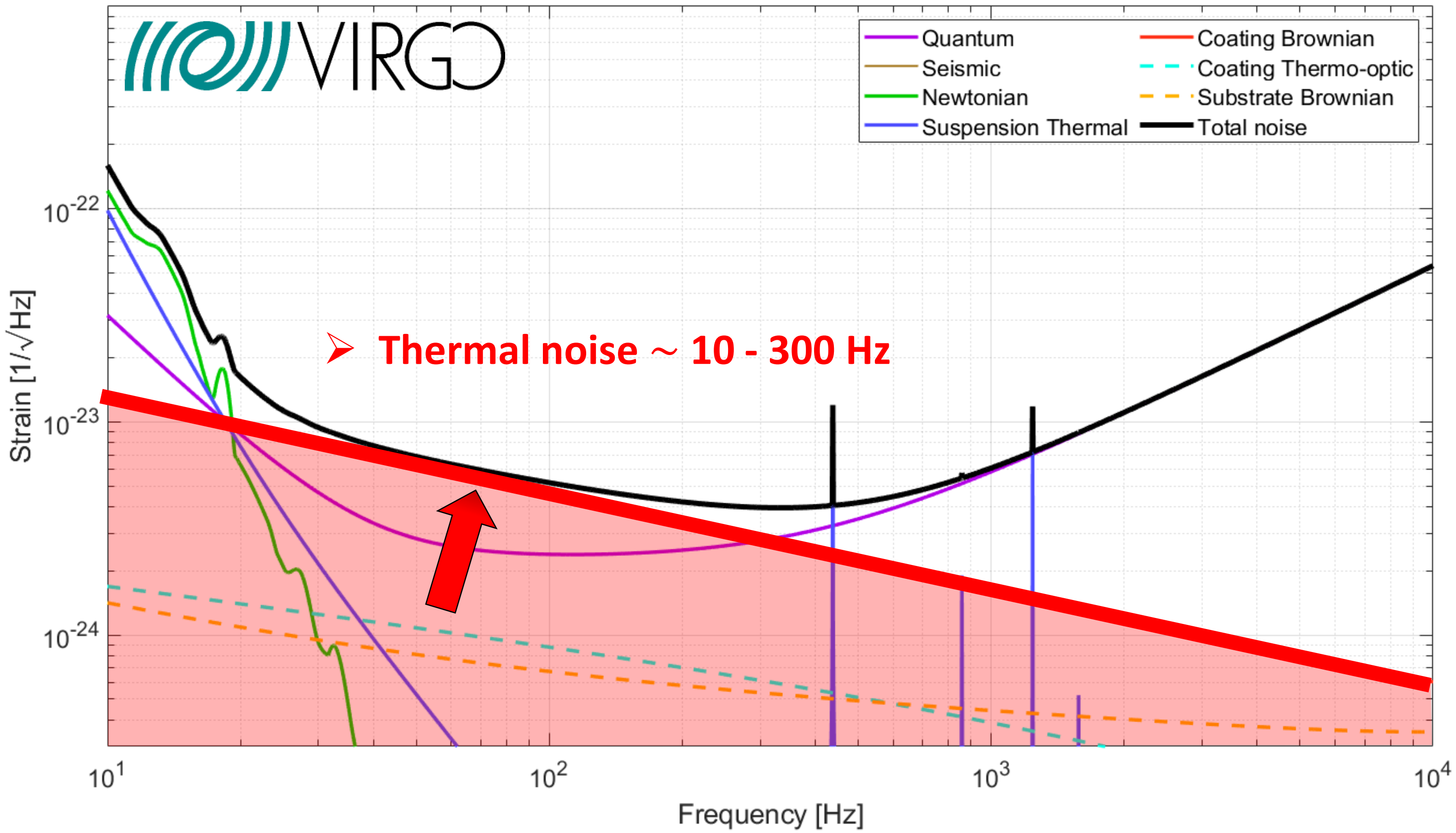
Coating Solutions Provider

Università di Roma Tor Vergata

Institut Lumière Matière

Thermal Noise

Project sensitivity curve



Temperature

Mechanical loss

Coating thickness

$$\mathrm{CTN}(f) \propto \frac{\sqrt{\frac{T}{f}\,\frac{1}{{w_b}^2}\,\varphi\, t_{coat}}}{L}$$

Beam-size

Arm length

Phase II upgrades:

Factor 3 reduction of coating loss angle

Beam size increase on ETM

Increase the mechanical performances *of today's reflective coatings,* ***retaining their outstanding optical and morphological properties.***

High Coordination Number Glasses: SiC

➢ *Mechanical properties*: linked to Two Level Systems (TLS) number density.

Reduction of total number of TLS

↓

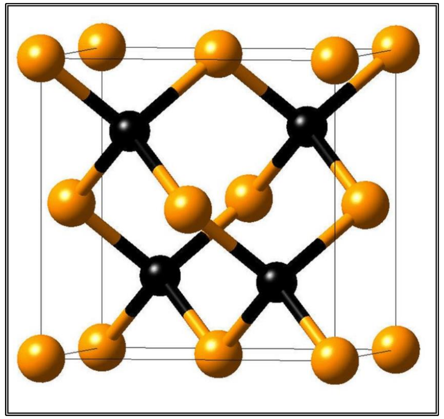
High coordination number glasses

↓

Coordination number is the number of atoms bonded to a central one: if it is **higher than 3**, the structure is more rigid (high coordination number materials are often linked via their edges or their faces making structural reorganization more difficult)

Low TLS density in high coordination number materials:

➢ SiC: mainly hexagonal coordination geometry of Si and C
  - Potentially of interest in several applications where high transparency needs to pair with good mechanical properties.
  - However a-SiC is a rather unexplored material.
  - Its properties may depend both in the composition and on the deposition methods.
  - The microscopic origin of its properties needs to be investigated.



Amorphous SiC samples

VIR-0913A-20

VIR-0077A-20

Thin Film Optics Group

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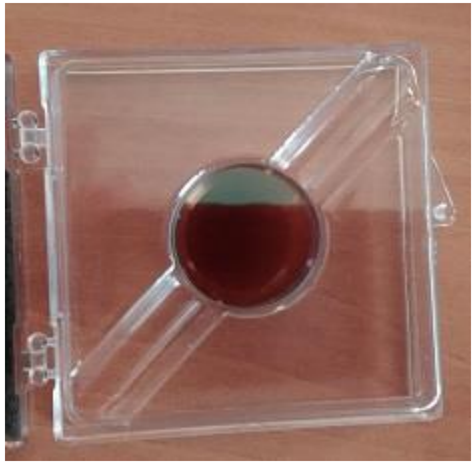
Coating Solutions Provider

1. **Ion Beam Sputtering (IBS) SiC**

❖ 3 samples produced @GOLD

- 1 x 100 nm [nominal thickness] on 1” Al_2O_3 witness sample
- 2 x 200 nm [nominal thickness] on each side of 2 “ SiO_2 disks

➢ SiC sputtering target purity = 99,9995%



INFN LNL

Istituto Nazionale di Fisica Nucleare

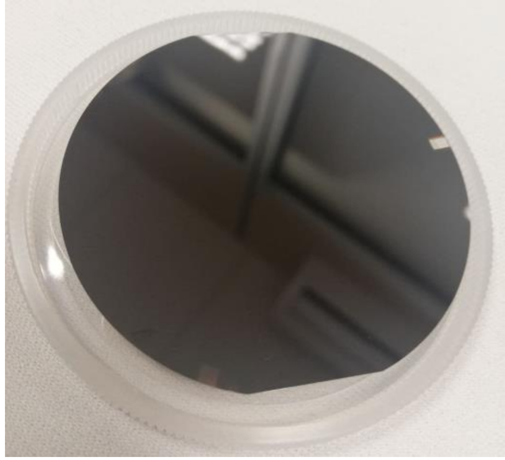
Laboratori Nazionali di Legnaro

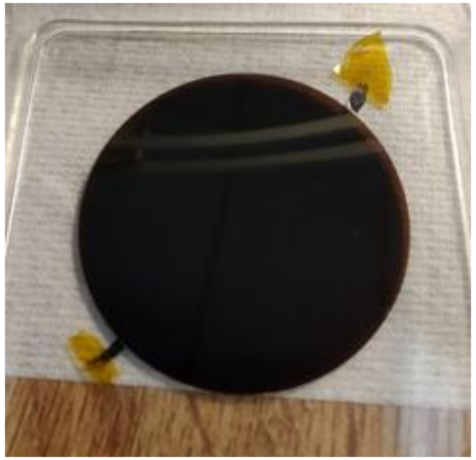
2. **Magnetron Sputtering (MS) SiC**

❖ Several samples produced @INFN-LNL

- 100 – 500 nm
- Different stoichiometries
- Different substrates (Si, SiO_2)

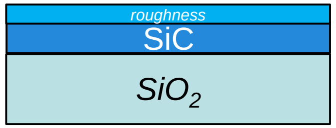
➢ SiC sputtering target purity = 99,999%



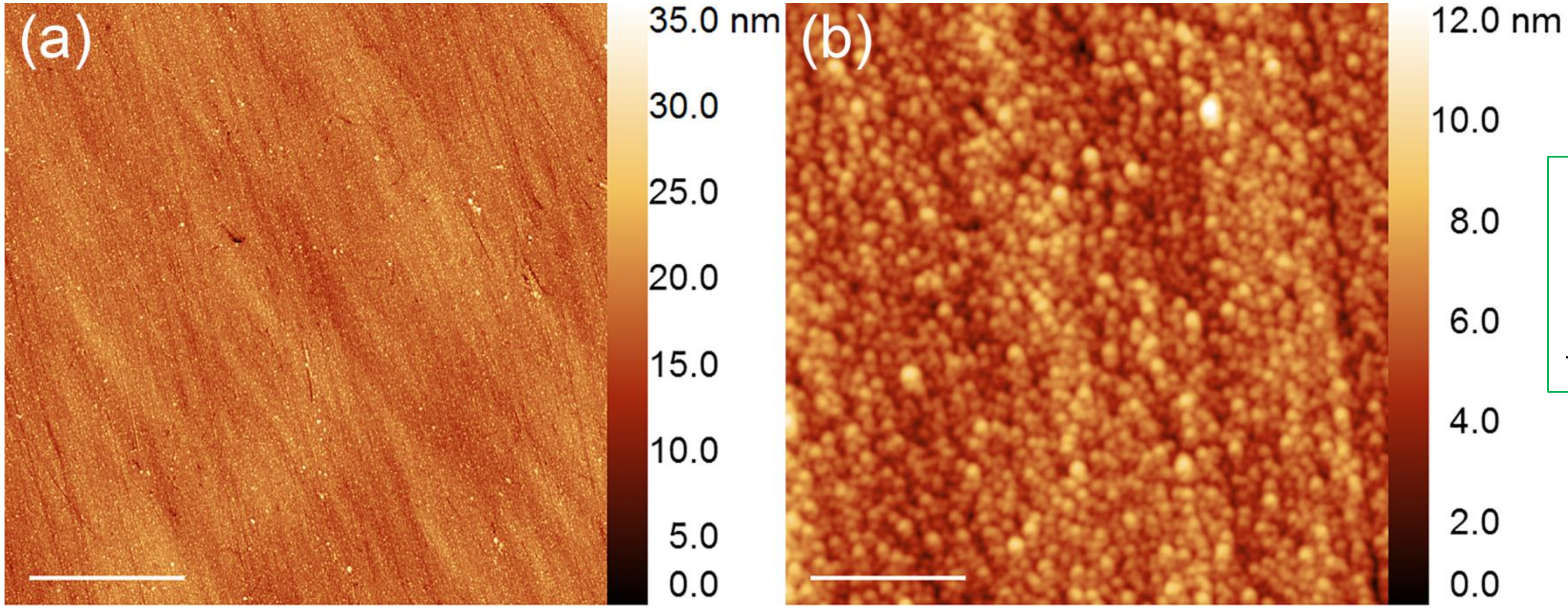


Morphological characterization

Sample: SiO_2 substrate t = 0.1 mm + **MS – SiC** coating 500 nm [nominal]   Si/C = 0.74



AFM topographies of SiC surface. The image scale-bars are respectively (a) 5µm and (b) 500 nm.

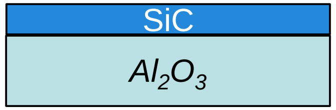


RMS Roughness = 2.25 nm

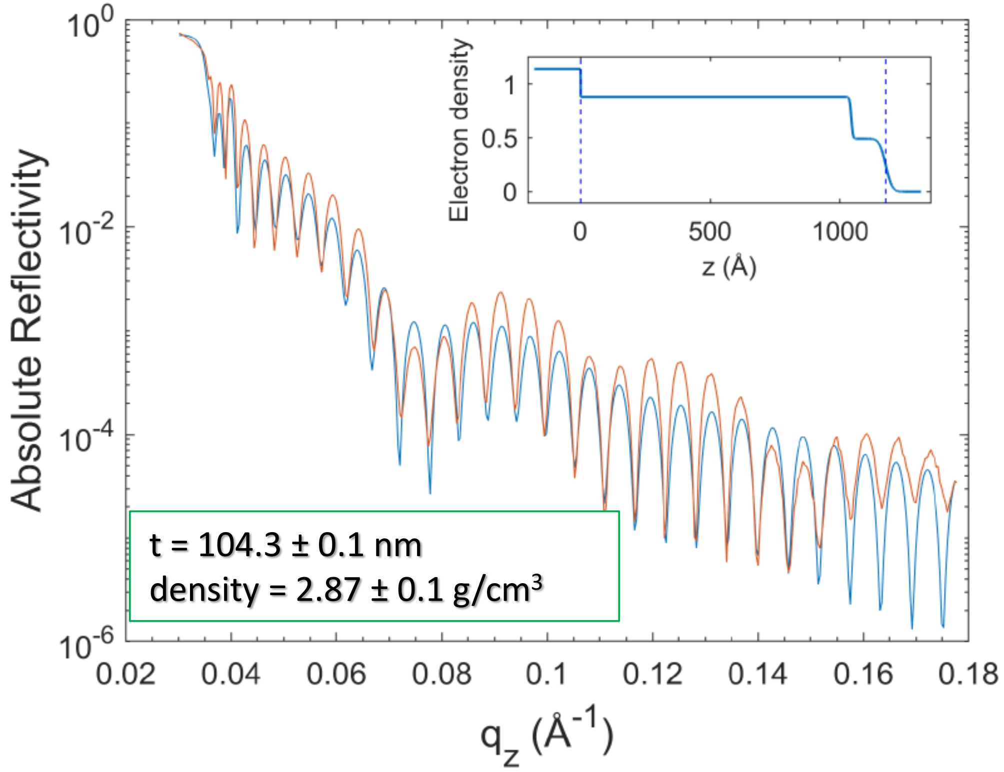
It seems to be present some raw textures (probably due to the polishing)

Structural characterizations

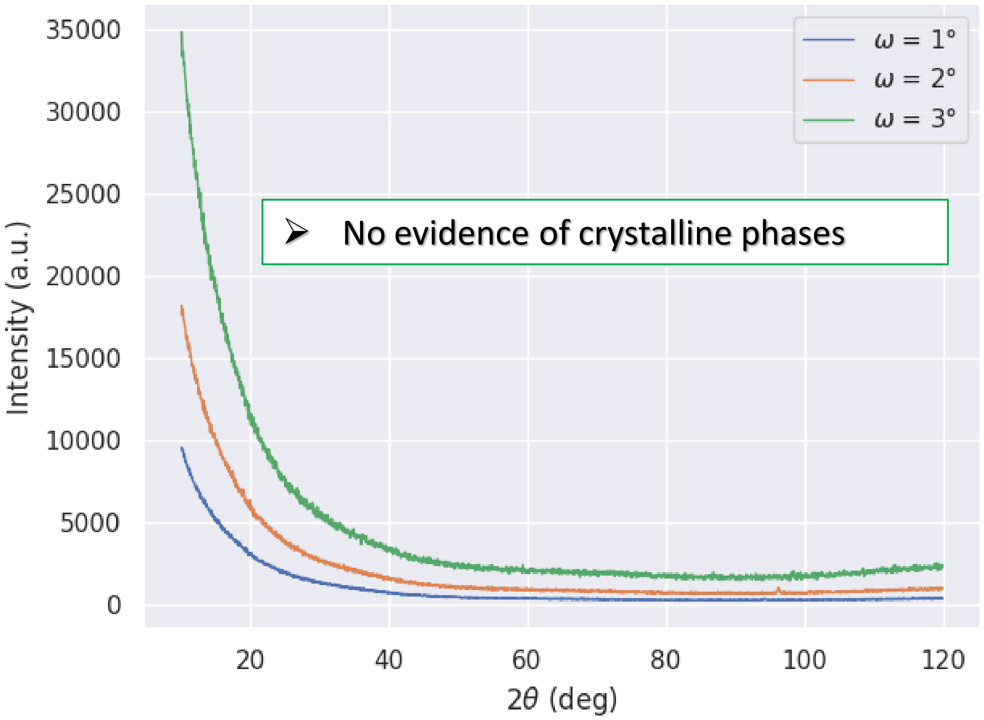
Sample: Al_2O_3 substrate 1" + **IBS – SiC** coating 104.3 nm



XRR analysis

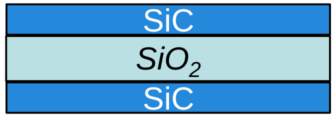


GI-XRD analysis

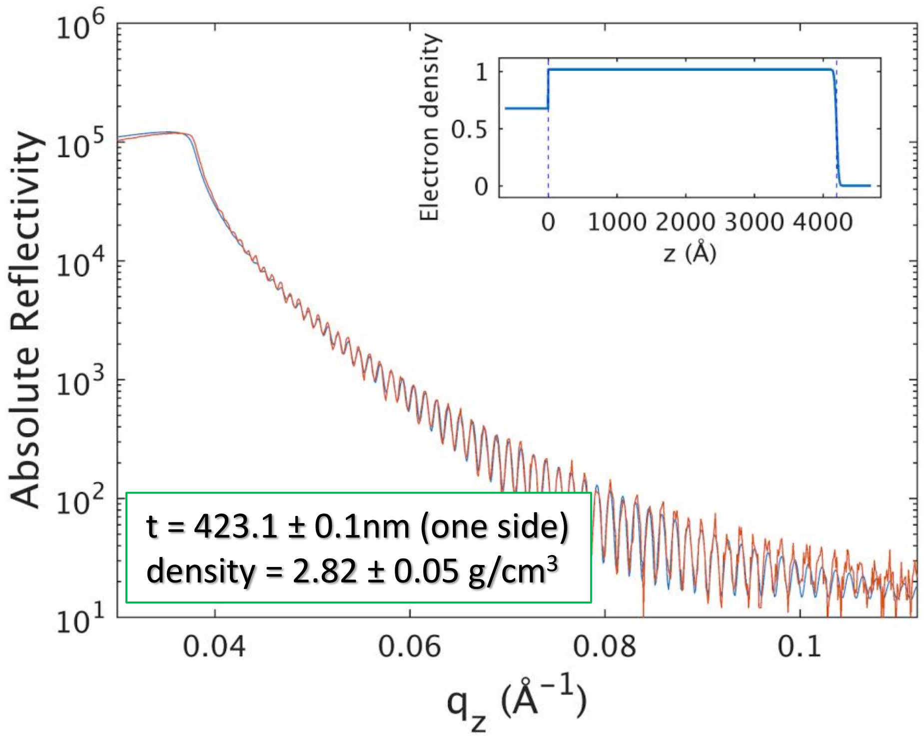


Structural characterizations

Sample: SiO_2 substrate 2” + **MS – SiC** coating 423.1 nm (on one side)

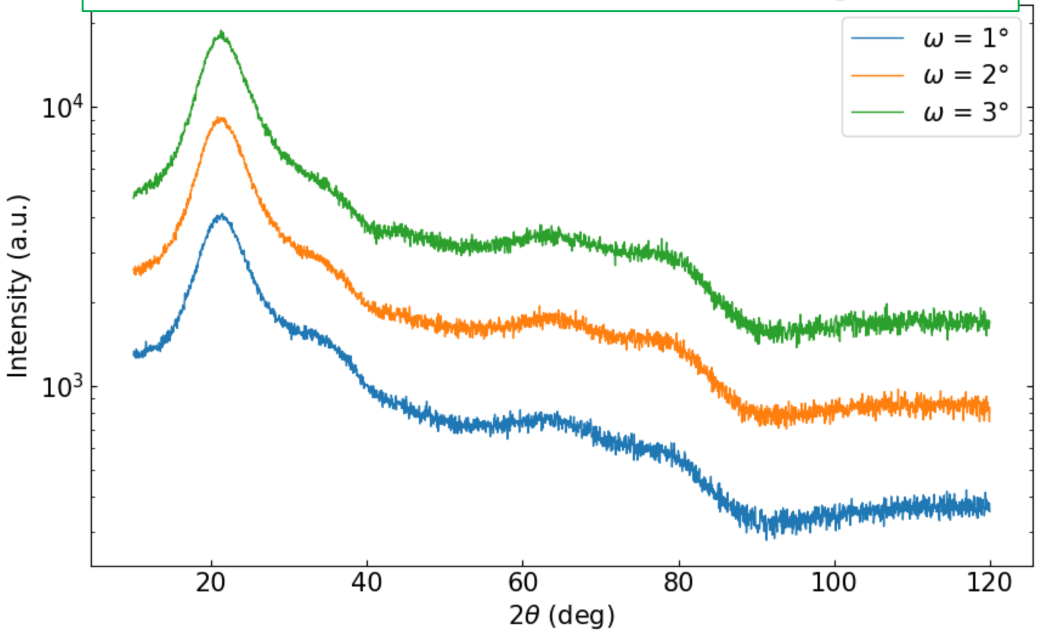


XRR analysis



GI-XRD analysis

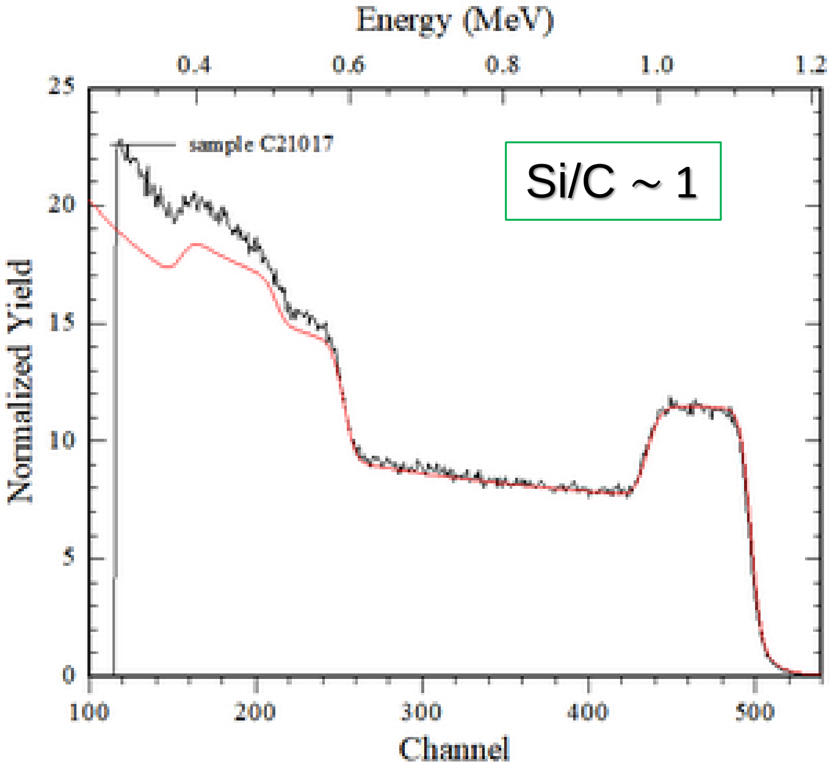
- No evidence of SiC crystalline phase
- Background structure due to underlying SiO_2 substrate



Composition characterization

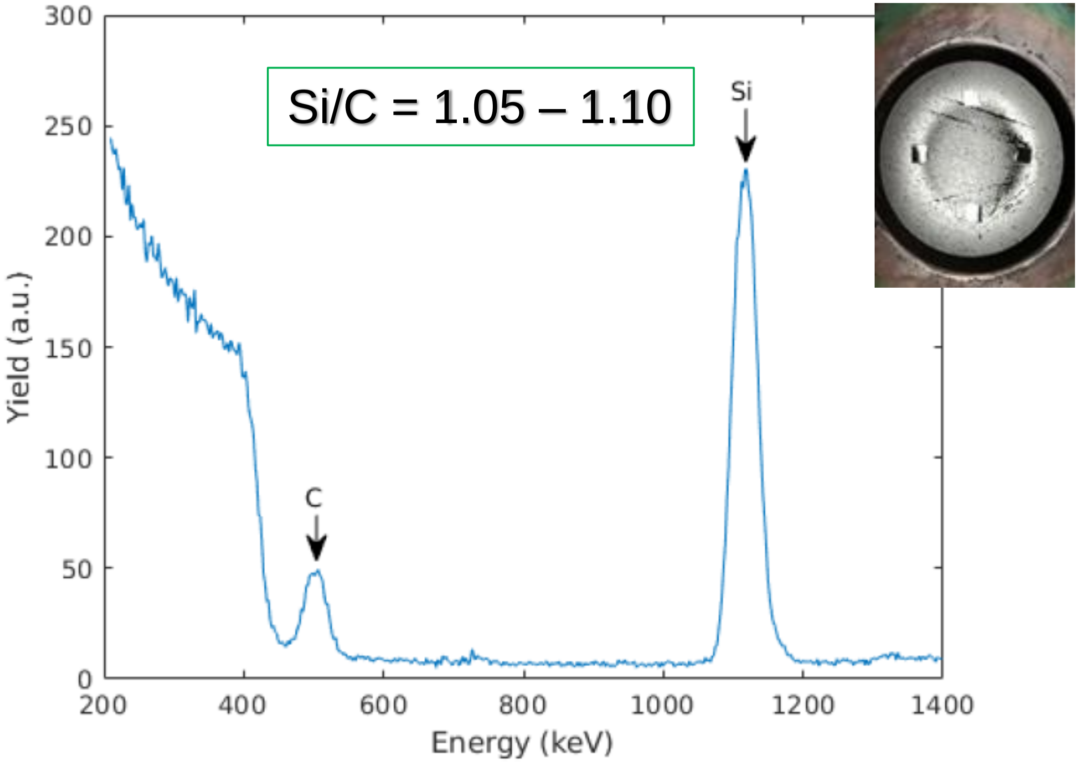
RBS analysis IBS – SiC

As-deposited IBS samples are close to the stoichiometric composition.



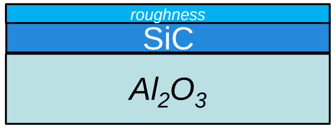
RBS analysis MS – SiC

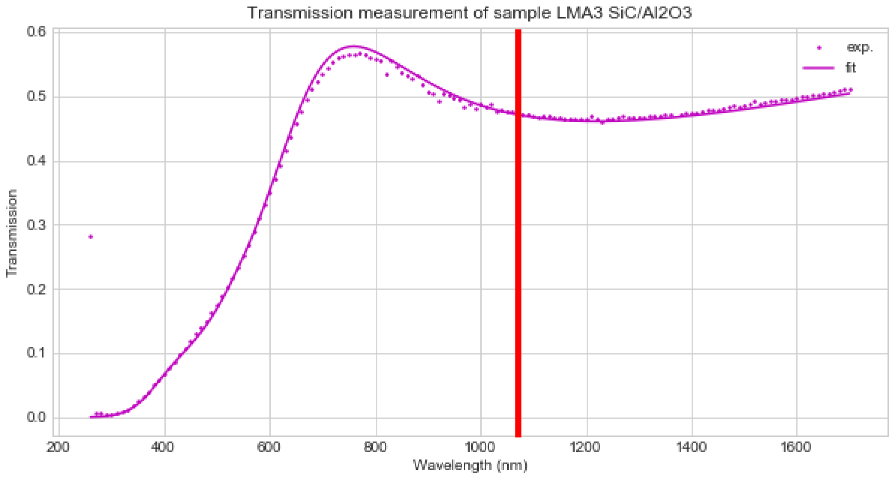
MS deposited samples are weak in Si (Si/C = 0.74). By adding some Si pieces on the target the composition can be tuned.



Optical characterizations

Sample: Al_2O_3 substrate t = 5 mm + **IBS – SiC** coating 101.59 nm Si/C = 1

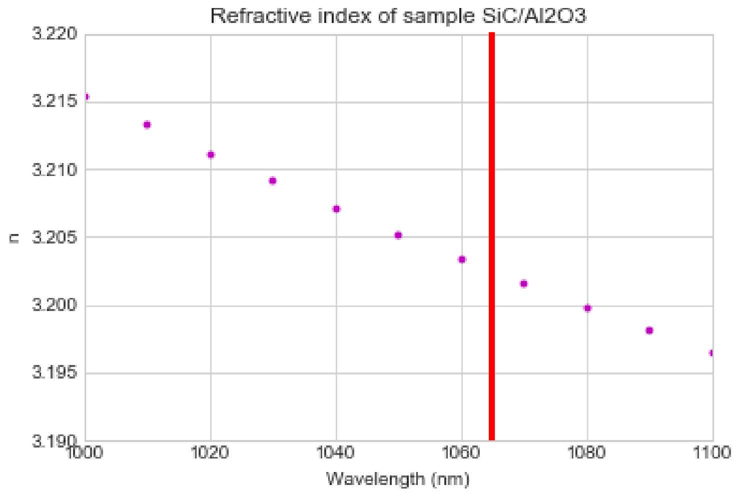


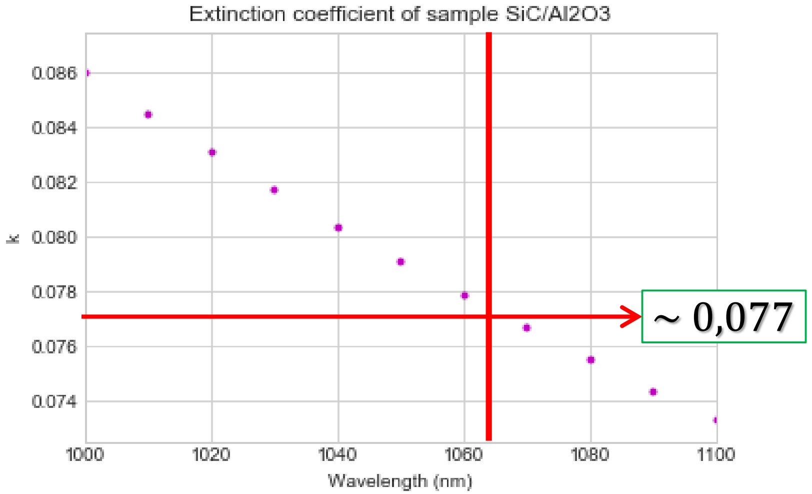


SE fit results

SiC: 101.59 ± 0.05 nm

OptRough: 1.50 ± 0.04 nm

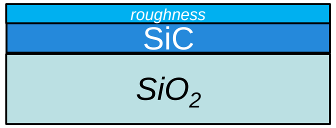


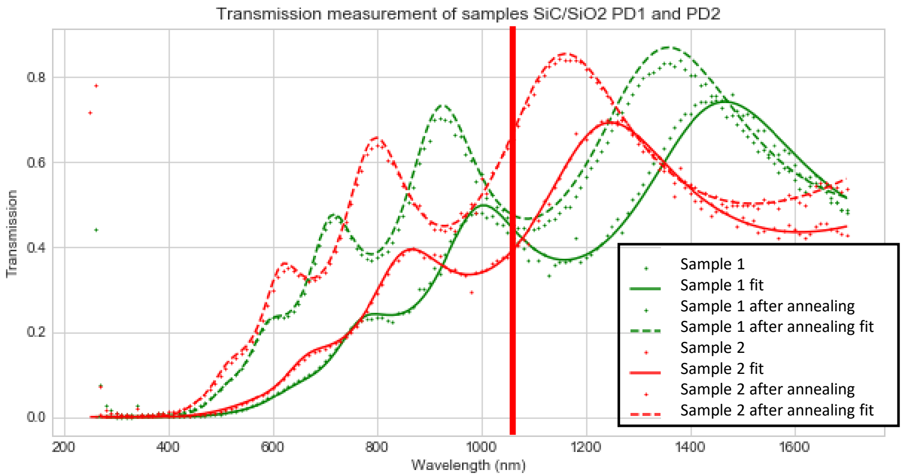


- First estimation of the absorption: it is way too high
  $k_{target} \sim 10^{-6}$

Optical characterizations

2 Samples: SiO_2 substrate t = 0.1 mm + **MS – SiC** coating 500 nm [nominal]   Si/C = 0.74

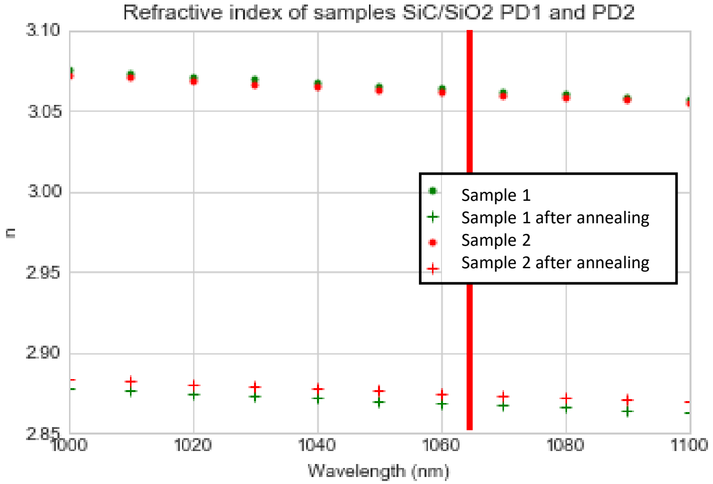


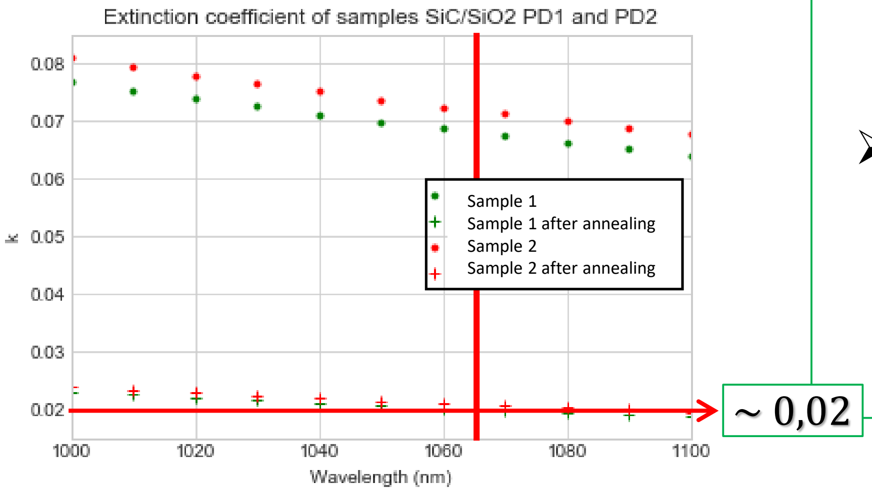


SE fit results

1. SiC: 478.8 ± 0.8 nm
   OptRough: 5.78 ± 0.16 nm

2. SiC: 401.8 ± 0.7 nm
   OptRough: 8.28 ± 0.19 nm

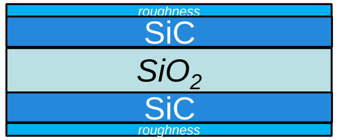




- ✓ The annealing reduces the absorption of about 5 times
- ➢ The absorption is still way too high $k_{target} \sim 10^{-6}$
- ➢ The stoichiometry does not seem to modify significantly the optical properties: further investigation ongoing!

Mechanical characterizations

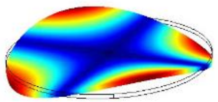
Sample:
SiO_2 substrate t = 0.5 mm
IBS – SiC coating 2x 220 nm



Resonant ring-down method and Gentle Nodal Suspension

Vibrating body (disc-shaped sample, properly suspended) damping characteristic time of free oscillation:

$$\varphi = \frac{1}{\pi f \tau}$$



Coating loss angle detection:

$$\varphi_{coat} \cong \frac{\varphi_{sub+coat} + (D-1)\,\varphi_{sub}}{D} \qquad \text{where: } D = 1 - \frac{m_0}{m}\left(\frac{f_0}{f}\right)^2$$

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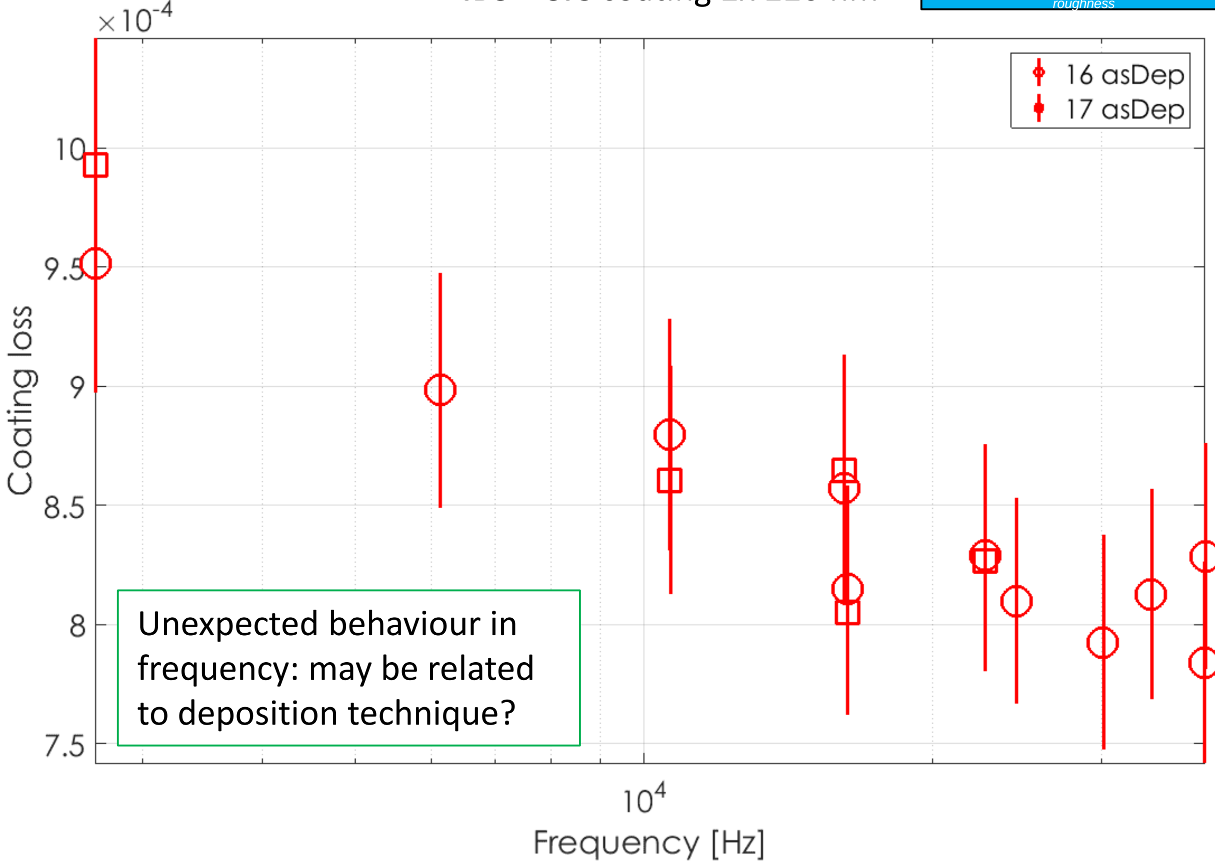
Procedure:
- f and f_0 measured
- m and m_0 measured
- φ_{sub} and $\varphi_{sub+coat}$



- ➢ $\boldsymbol{\varphi_{coat} = [7,5 - 10,0] \times 10^{-4}}$
- ➢ $\boldsymbol{Y = 274 \pm 1}$ **GPa**
- ➢ $\boldsymbol{\upsilon = 0,21 \pm 0,01}$

➢ Open issue: density $\boldsymbol{\rho = 2,25 \pm 0,8}$ **g/cm3**
Measured thanks to SE measurements of thickness = 220 ± 5 nm

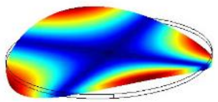
Mechanical characterizations

Università di Roma Tor Vergata

Resonant ring-down method and Gentle Nodal Suspension

Vibrating body (disc-shaped sample, properly suspended) damping characteristic time of free oscillation:

$$\varphi = \frac{1}{\pi f \tau}$$



Coating loss angle detection:

$$\varphi_{coat} \cong \frac{\varphi_{sub+coat} + (D-1)\,\varphi_{sub}}{D} \qquad \text{where:} \quad D = 1 - \frac{m_0}{m}\left(\frac{f_0}{f}\right)^2$$

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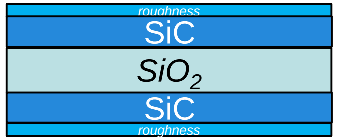
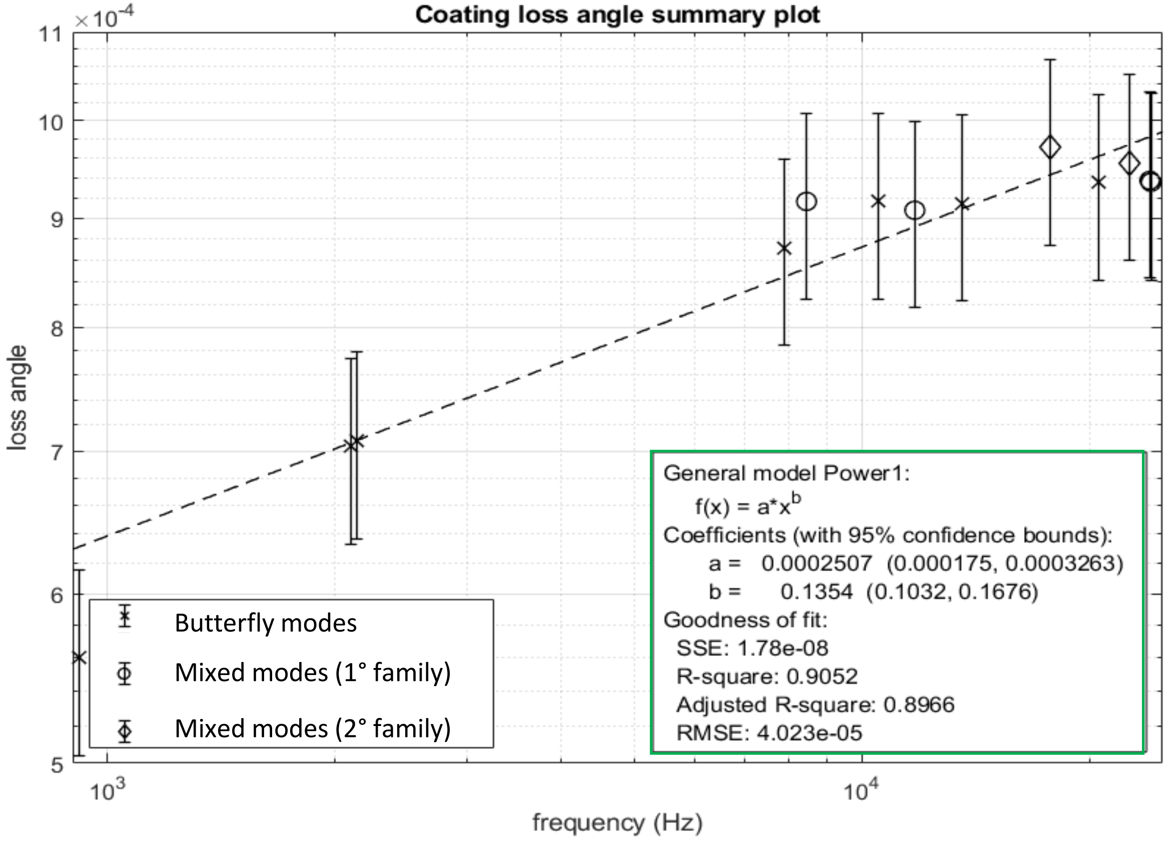
Procedure:

- f and f_0 measured
- m and m_0 calculated (thanks to SE measurement of the coating thicknesses and XRR measurement of density)
- φ_{sub} and $\varphi_{sub+coat}$

> ➢ $\boldsymbol{\varphi_{coat} = [5 - 11] \times 10^{-4}}$
> ➢ ***Y* and *υ* still to be evaluated**

Sample:
SiO_2 substrate t = 0.35 mm
MS – SiC coating 431 + 422 nm





Molecular Dynamic simulations

VIR-0379A-21

Model from "*Vashishta et al*, JAP **101**, 103515 (2007)": 2-body (repulsion, screened Coulomb, charge-dipole, van der Waals) and 3-body interactions (bond bending and stretching).

Benchmark on crystalline and liquid SiC: good agreement with exp data.

Preparation of the amorphous samples via melt cooling (zero pressure).

Strong tendency to crystallize, tuning the cooling rate crystallized fraction (CF) in the range 10% or less.

<u>Simulated amorphous-SiC:</u>

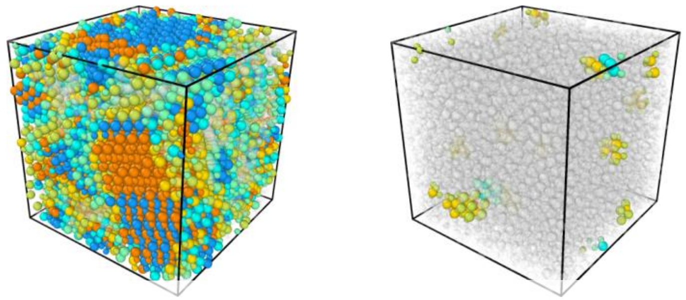
Density ρ = 2.98 g/cm^3

Young modulus E = 150 ± 10 Gpa

Poisson's ratio ν = 0.29 ± 0.01

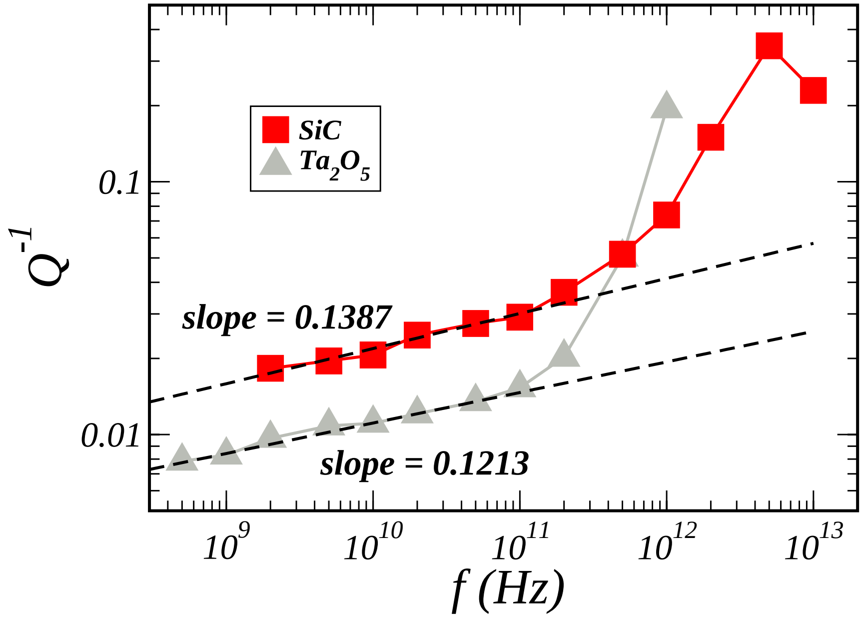
Rate 10^4 K/ns

Rate 10^5 K/ns



CF: 50-80%

CF <5%



- ➢ Density in good agreement with observed experimental values
- ➢ Poor agreement for mechanical properties

Conclusions

- No evidence of crystalline phases: **IBS and MS SiC samples are amorphous**
- Roughness from AFM and SE in agreement: $\sim [\mathbf{2}\ -\mathbf{10}]$ nm
- Density evaluation in agreement with literature and MD simulations: $\sim [\mathbf{2,8}\ -\mathbf{2,9}]$ **g/cm³**
- The absorption is still way too high [wrt $\sim 10^{-6}$ desired value]: $\mathbf{k} \sim \mathbf{2} \times \mathbf{10^{-2}}$ (after annealing)
- IBS and MS SiC loss angle values in agreement: $\boldsymbol{\varphi} \sim [\mathbf{5}\ -\mathbf{11}]\ \times \mathbf{10^{-4}}$
- Elastic and mechanical properties not in agreement with literature and MD simulations

➢ Reasons for the strong absorption still to be understood

  ➢ Direct measurement may give better estimation, rather than SE (less sensitive at that wavelength and depending on many fit variables)

➢ Investigation of stoichiometry: any correlation with the observed properties? Ongoing!

➢ Investigate possible reasons to explain the discrepancy with respect to MD simulations

Thank you!

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Wednesday, 19 May

06:00 → 08:00 **Coating thermal noise Workshop: Hour 3-4**

Conveners: Elisabetta Cesarini (ROMA2) , Gianpietro Cagnoli (ILM-UCBL) , Stuart Reid (SUPA, University of Strathclyde)

06:00 **Coating choice for O5: Summay** 15m

06:15 **Coating choice for O5: Discussion** 30m

06:45 **Metrology open issues in GeNS measurements** 15m

The Gentle Nodal Suspension (GeNS) has become the most common technique for measuring coating mechanical dissipation, showing an unprecedented result repeatability on disk shaped substrates. GeNS gives the possibilities to perform measurement so accurate that it is possible to follow even tiny changes in the sample mechanical behavior. The high level of sensitivity makes some new systematic effect to be relevant, posing metrological issues which are currently unsolved.
Sample curvature changes caused by non symmetrical coatings and post-deposition thermal treatments, and changes of few degrees in sample temperature, produce mode frequency shifts which overlap to the ones given by the coating itself. This overlapping spoils the accuracy of dilution factor measurement and elastic parameters estimation.
Dissipation of silicon and sapphire substrates, commonly used in cryogenics measurements, are dominated for most of the temperature span by thermoelastic damping. Changing in the thermoelastic dissipation is shown to be induced by coating deposition. Since coating loss angle is measured by difference, this effect gives a systematic error in assuming bare substrate not altered by deposition. Lastly both the thermoelastic damping shift, as well as the dishomogeneity of the coating at the sample edge, can give systematics in trying to disentangle different bulk and shear loss angles. A description of these open issues will be given and a path for solutions will be presented.

Speaker: Francesco Piergiovanni (Istituto Nazionale di Fisica Nucleare)

07:10 **Properties of amorphous SiC films** 5m

The observational horizon of interferometric gravitational wave (GW) detectors is limited by thermal noise in the coating at mid-range frequency, where first GW signals have been detected and many others are expected. The main responsible are the intrinsic dissipations, intimately linked to the inelastic behaviour of the amorphous coating materials. This behaviour is generally explained by the presence of a number of metastable atomic configurations of the amorphous matrix which can switch between two different states by thermally activated processes. Any two of these states that are separated by an energy barrier is called a two level system (TLS). In order to reduce the dissipation of amorphous materials two basic ideas can be pursued: a reduction of the total number density of TLS or an optimal distribution of TLS. Depositing amorphous film of materials whose coordination number is superior to three should lead to a low number of TLS.
Among the candidate high coordination number glasses, we investigated amorphous SiC, interesting for advanced applications and still lacking a deep study. Here are presented structural, chemical, optical and mechanical characterizations of a-SiC films, deposited by Ion Beam Sputtering and Magnetron Sputtering techniques. Furthermore, molecular dynamic simulations to evaluate elastic properties in a wide energetic range are shown.

Speaker: Diana Lumaca (Università di Roma Tor Vergata e INFN Sezione di Roma Tor Vergata)

07:20 **Optical and mechanical characterization of ion-beam-sputtered MgF2 and AlF3 thin films** 5m

GW detector highly reflective coatings are obtained by alternate layers of material with different refractive indexes. Brownian thermal noise associated with the coating stack, limits the mid-frequency region of the GW detector designed sensitivity. Thermal noise reduction can be achieved minimizing the overall thickness of the stack, increasing the refractive index contrast . Fluoride's coatings, largely used in UV application, show the lowest measured values of refractive index, and they can be interesting for future GW detectors as low index material. The first optical and mechanical characterization of ion-beam-sputtered MgF2 and AlF3 thin films has been performed, starting the investigation on the possible utilization of fluorides in future GW detectors. Methods and results will be described, effects of post deposition thermal treatments will be presented.

Speaker: Matteo Bischi (Istituto Nazionale di Fisica Nucleare)