

Atomic structure investigations of amorphous coatings

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Introduction

Reducing coating thermal noise is key challenge for future detectors



- Number to beat:
 - Mechanical loss Ti: $Ta_2O_5 = 2 \times 10^{-4}$
- Changes in mechanical loss are the result of changes in atomic structure
- Measure structure at the short (< 0.5 nm) and medium range (> 0.5 nm)

aLIGO noise budget (GWIN



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Tantala: order and disorder

					Ta - (С
High-P	Zibrov (C 1 2 1)				,	
	Zibrov (C 1 2/c 1)		Ĩ		 	
	Zibrov (I b a m)			Τ		
	Perez-Walton (C 1 2/c 1)				 	
	Perez-Walton (C 1 2/c 1)				 	
High-T	Liu (A 1 2/m 1)				 	
	Liu (I m m a)				 	
	Liu (I 41/a m d S)	-			 	
	Stephenson (I 1 2 1)					
Low-T	Lehovec (C 2 m m)		!			
	Hummel (P 2 m m)					
	Stephenson (P 2 m m)	i				
	Aleshina (P c c m)					
	Demont (P c c m)					
	Schmid (C m m m)		1		 	
	Lee, λ (P b a m)		1		 	
	1		2		3	





[R Bassiri et al, APL Materials, **3**, 036103 (2015)]



Tantala: order, disorder and mixing



[R Bassiri et al, Acta Mat., **3**, 036103 (2015)]





- Vibrational modes of primary structural units :
- Zr dopant suggested to make structure more flexible
- Experimental results underway at least as good as Ti:Ta₂O₅
- Si and Mg suggest to make sample more rigid potentially reducing RT loss



Measurement techniques: GI-XPDF: Grazing Incidence X-ray Pair Distribution Function







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Measurement techniques: FEM: Fluctuation Electron Microscopy











[M. Hart et. al., J. Non-Cryst. Solids, **438** 10 - 17 (2016)]







Tantala: GI:XPDF





[B Shyam et al, under review]



Tantala: GI:XPDF

- Modeling medium range order:
 - Extend primary structural unit
 - Suggests existence of rings similar to SiO₂ structure
- MRO important to understanding loss mechanisms





[B Shyam et al, under review]





Tantala: FEM



Stanford University





Where to next?

- Near term:
 - Medium range order in theoretical studies vs. experiment
 - Work with Hai Ping Cheng at U Florida to incorporate MRO to loss modeling
- Medium term:
 - Combine experimental to data to better constrain models
- Ultimate aim: develop a predictive tool for lower thermal noise coatings



Test materials which could have lower loss from predictions (Mg, Si doped tantala)

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Annealed and Zirconia doped





[B Shyam et al, under review]

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