"Phonons" and "Phasons" in icosahedral quasicrystals (i-QCs) and related approximant phases

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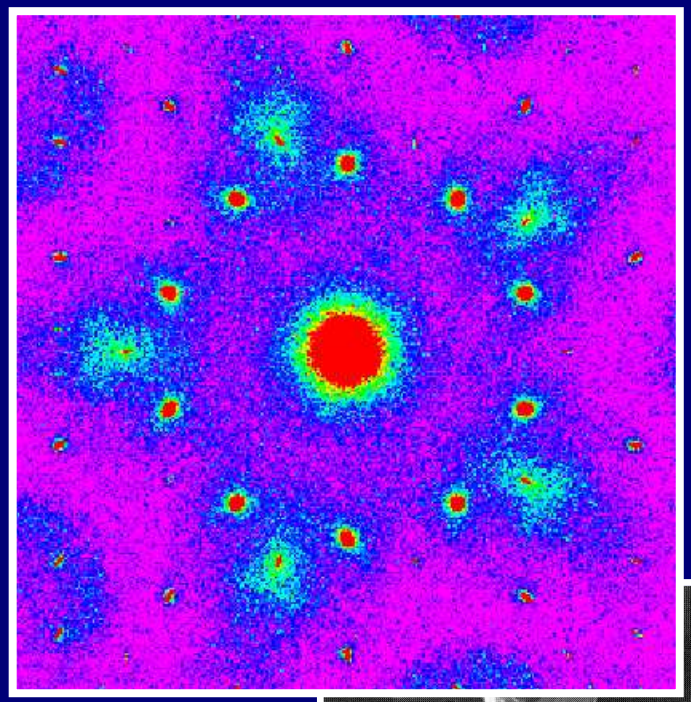
"What is a quasicrystal, what is an approximant"

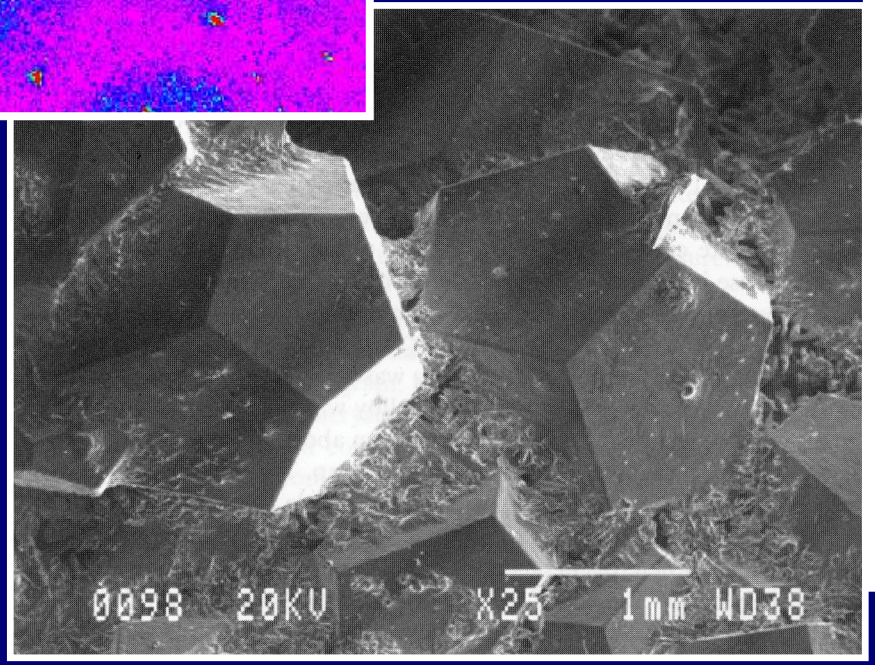


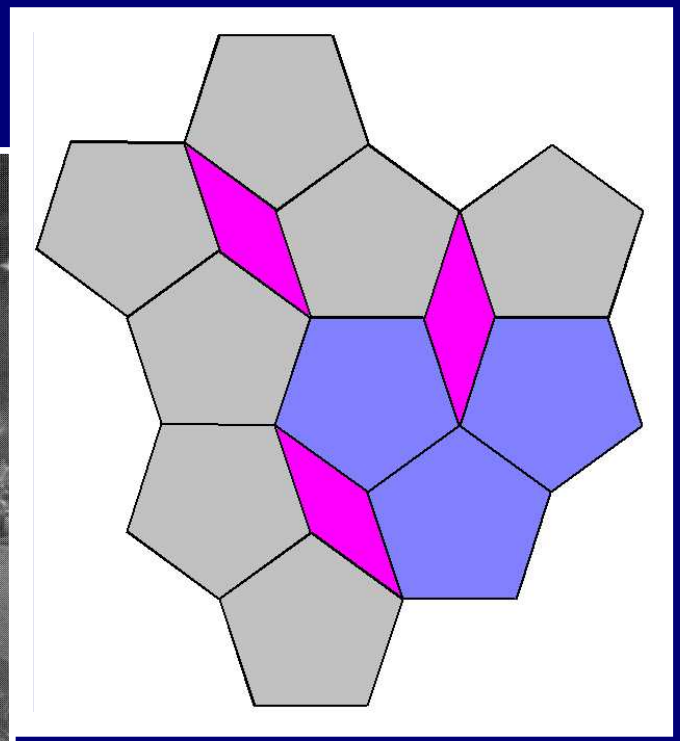
1984

Quasicrystals are intermetallic alloys (usually Zn- or Al-based)

" perfectly" long-range ordered but **NOT PERIODIC**

(forbidden 5-f symmetries for i-QCs)

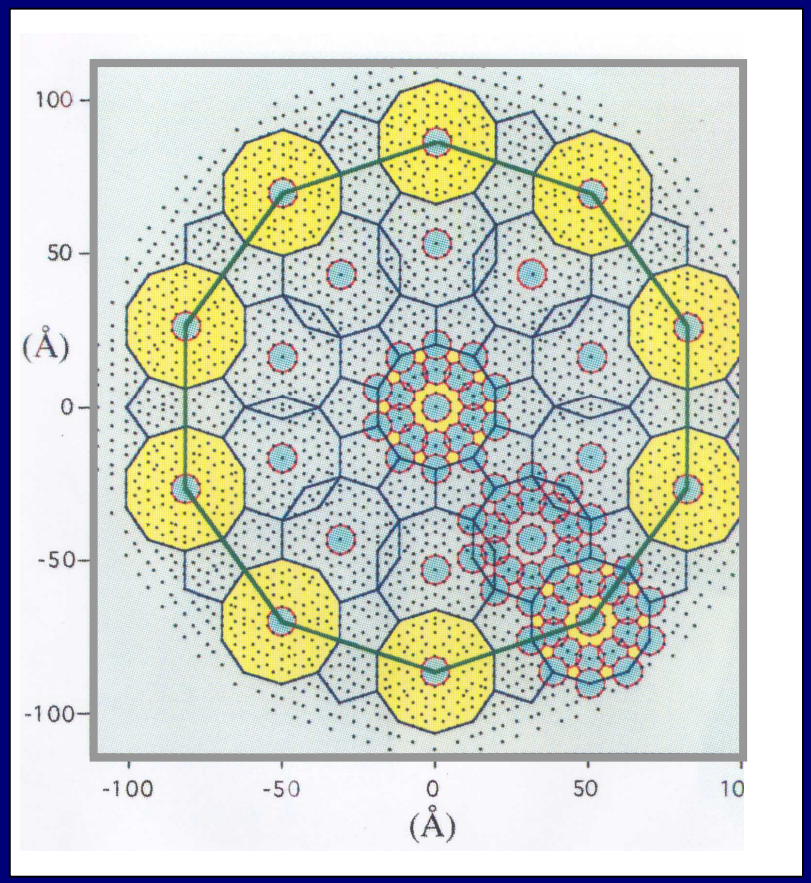




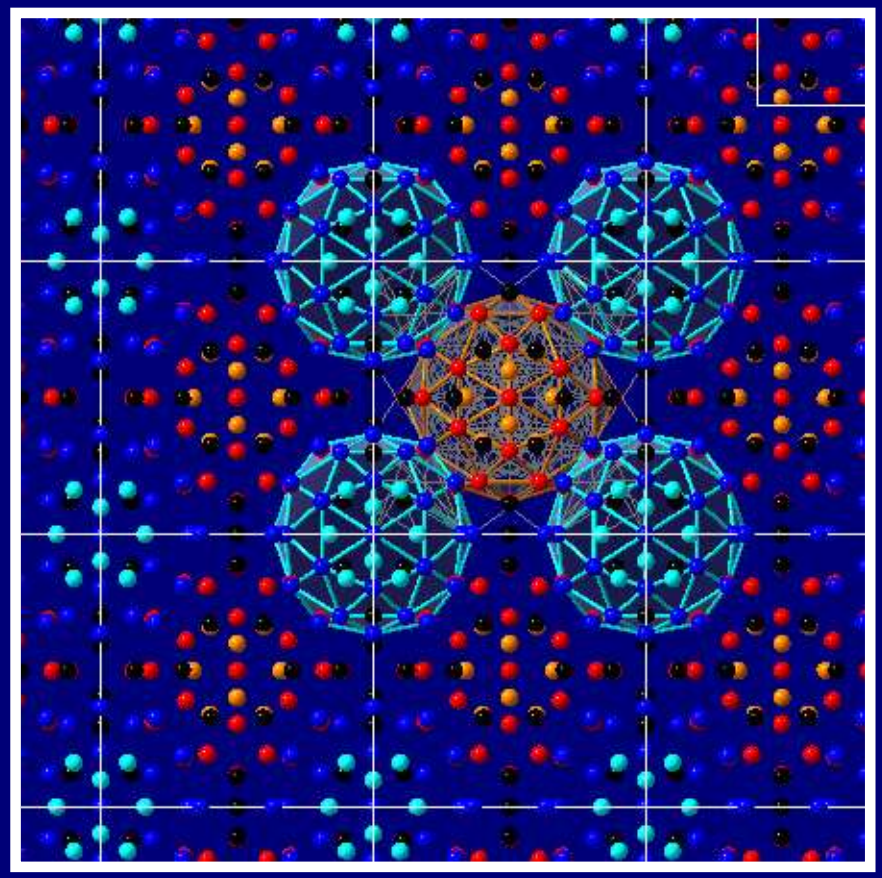
"What is a quasicrystal, what is an approximant"

Ordered compact packing of the same icosahedral clusters

QCs : autosimilarity and hierarchical packing of i-Clusters



1/1 Approximants : periodic packing of i-Clusters



Our motivations :

1) What is specific to the Quasiperiodicity in the dynamical response of a QC ?

2) What kind of atomic vibrations in a QC ? ⇒ calculations ⇒ periodicity

Our approach : "comparing the dynamics in systems of increasing complexity"

Structure	Mackay-type	Bergman-type	Tsai-type
Dynamics in the QC phase	yes : i-AlPdMn	yes : i-ZnMgY	X
Dynamics in the approximant phase	~no	no	X

Comparing different QCs : if differences, signature of the local order

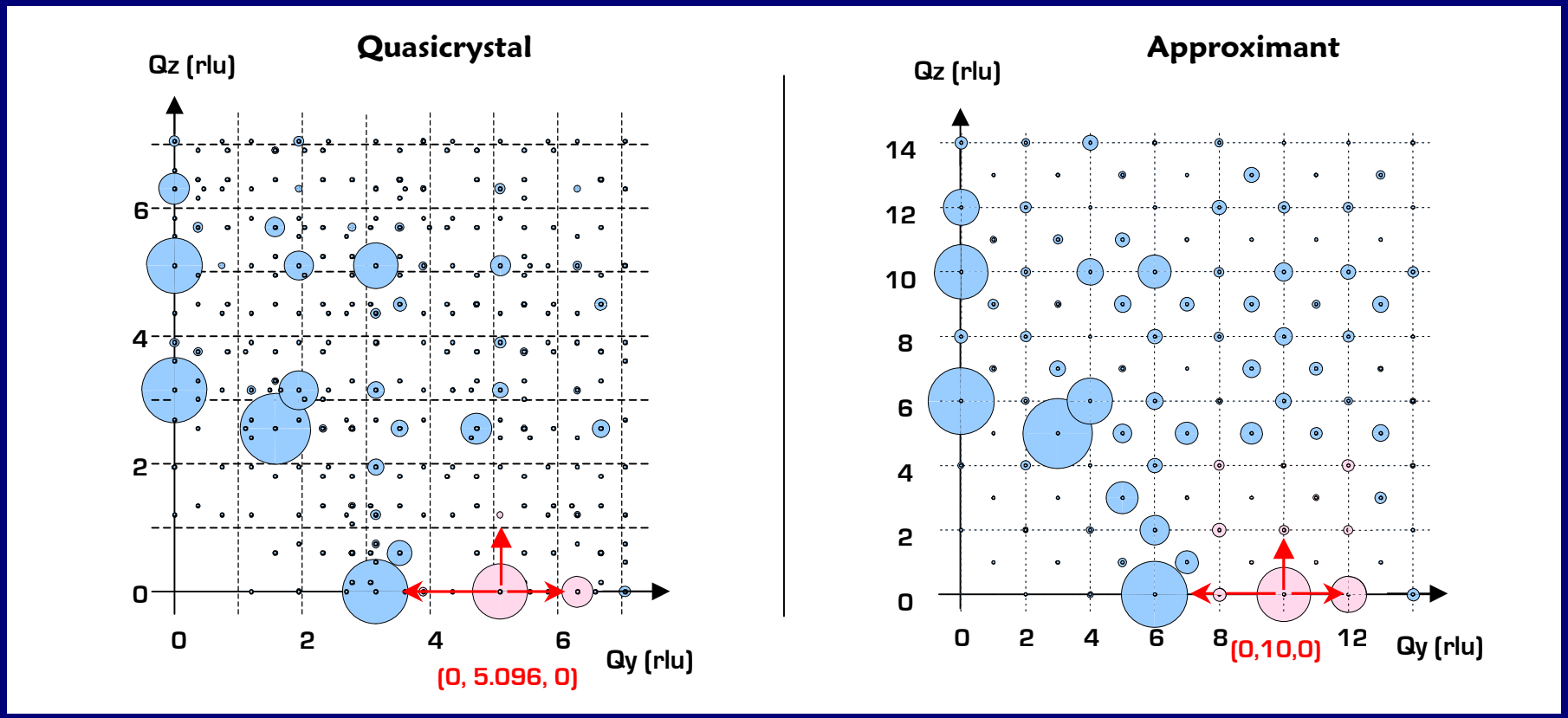
Comparing QCs and approximants : if differences, signature of the long-range order

Approximant phases are already complex crystalline phases with more than 150 atoms in the unit cell

What about the dynamics in « simplest » crystalline phases ?

"Phonons" in i-QCs and related approximant phases

Reciprocal space

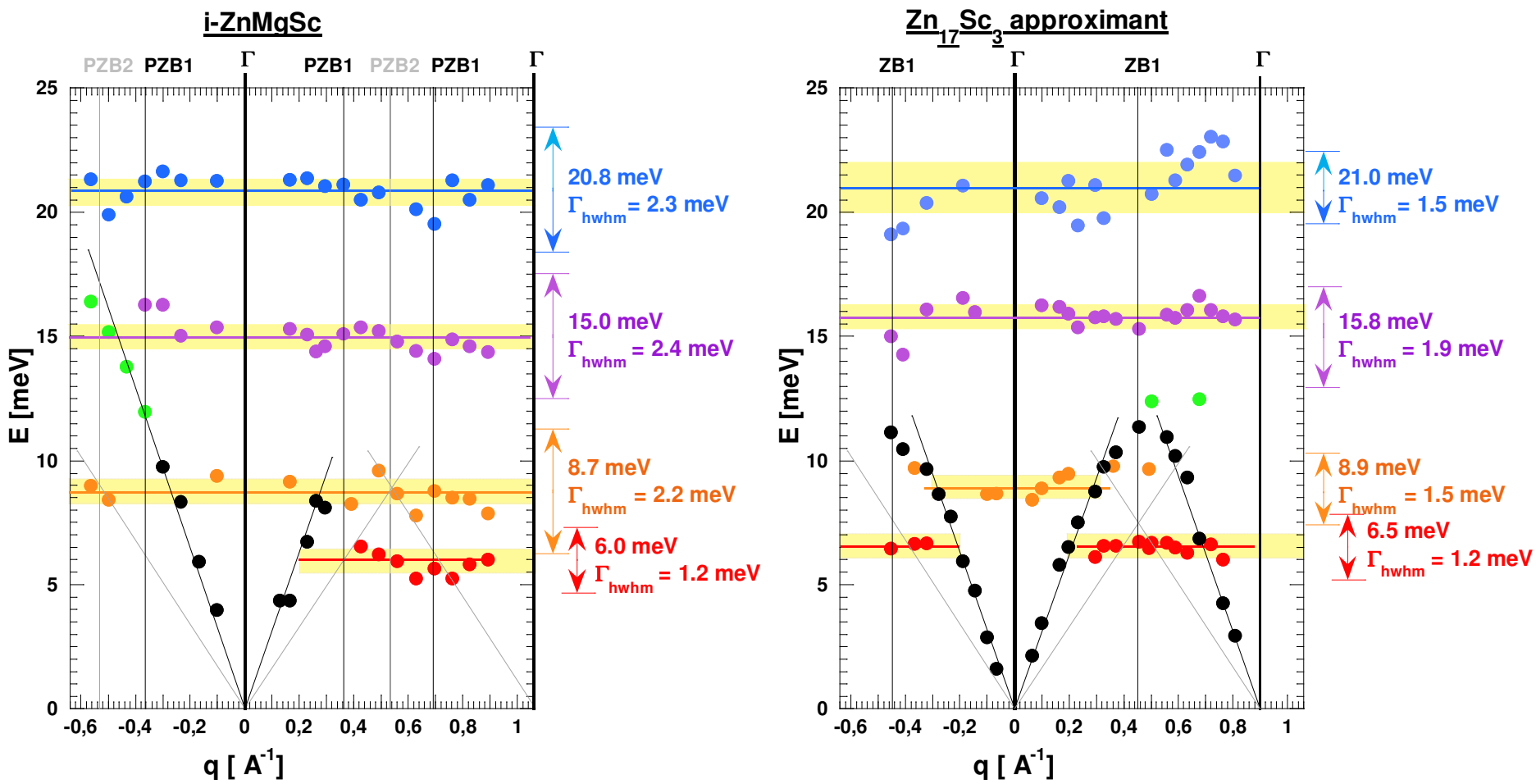


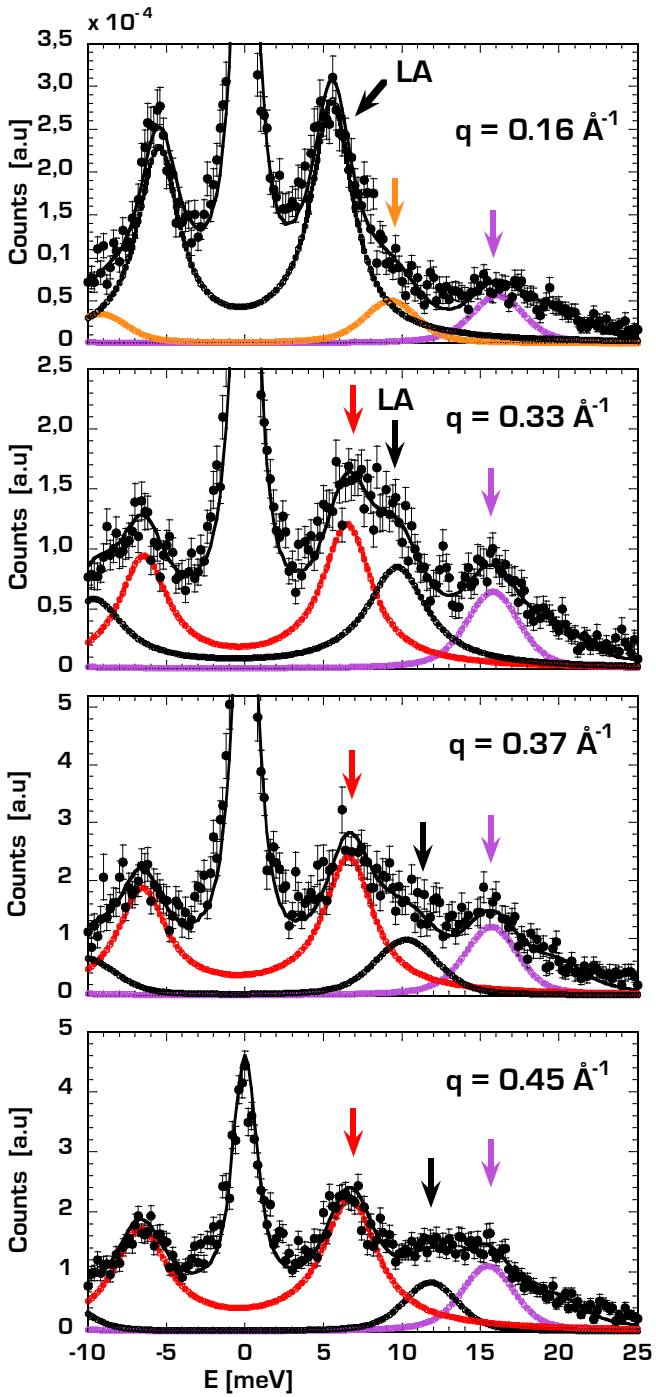
- different (quasiperiodic vs periodic) long-range orders

- similar distribution of the x-ray Bragg intensities : direct signature of similar local environments

Dynamics of "Phonon dynamics" in the i-ZnMgSc QC and its 1/1 ZnSc approximants : longitudinal modes

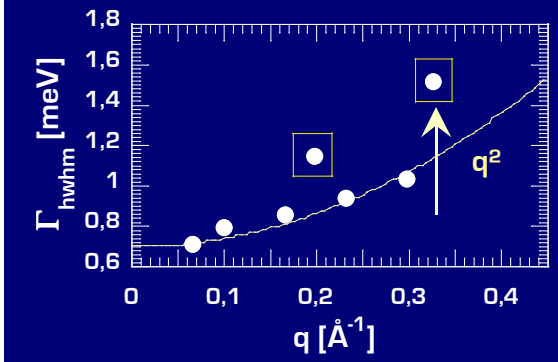
ν_{LA} = 5060 m.s^{-1}, ν_{TA} = 2600 m.s^{-1}





Lattice dynamics in the 1/1 $Zn_{17}Sc_3$ approximant

Longitudinal Acoustic modes



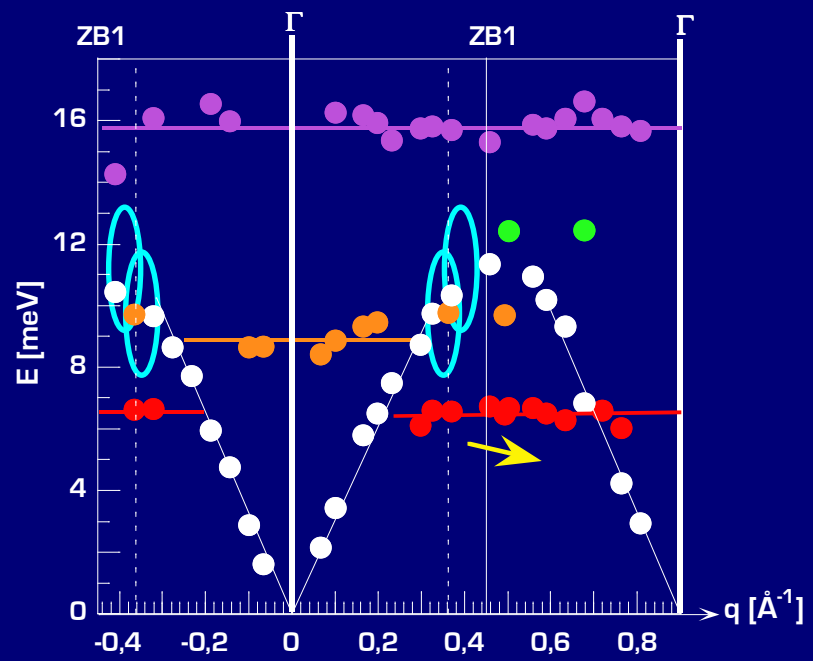
q ∈ [0, 0.33 Å^{-1}] :

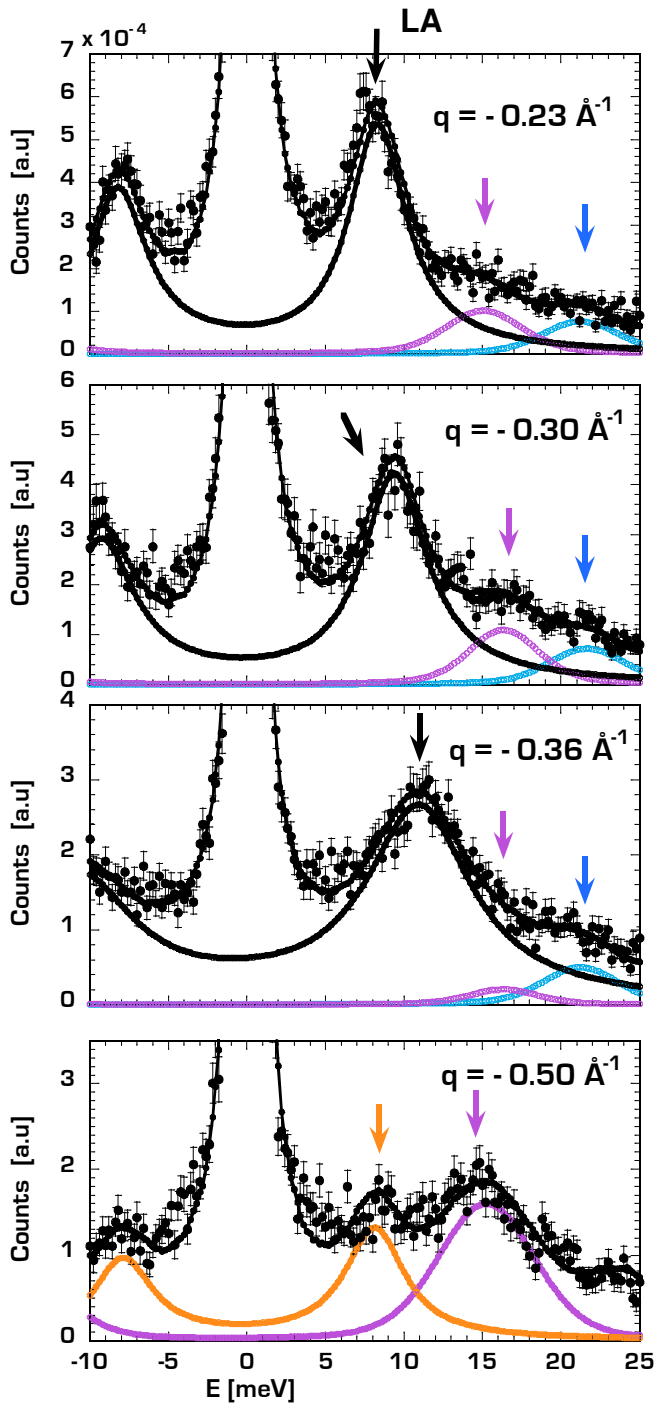
Smooth evolution of the width

anomalies when crossing optic bands

⇐ **q ∈ [0.33 - 0.37 Å^{-1}] :** Classical bending of the acoustic branch with strong intensity at the limit with the optic regime

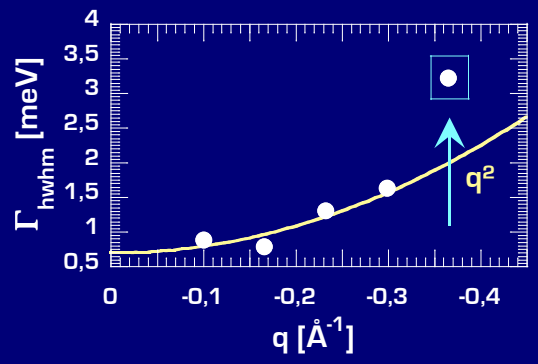
q > 0.45 Å^{-1} : spectral response dominated by the optic band at 6 meV





Lattice dynamics in the i-ZnMgSc quasicrystal

Longitudinal Acoustic modes



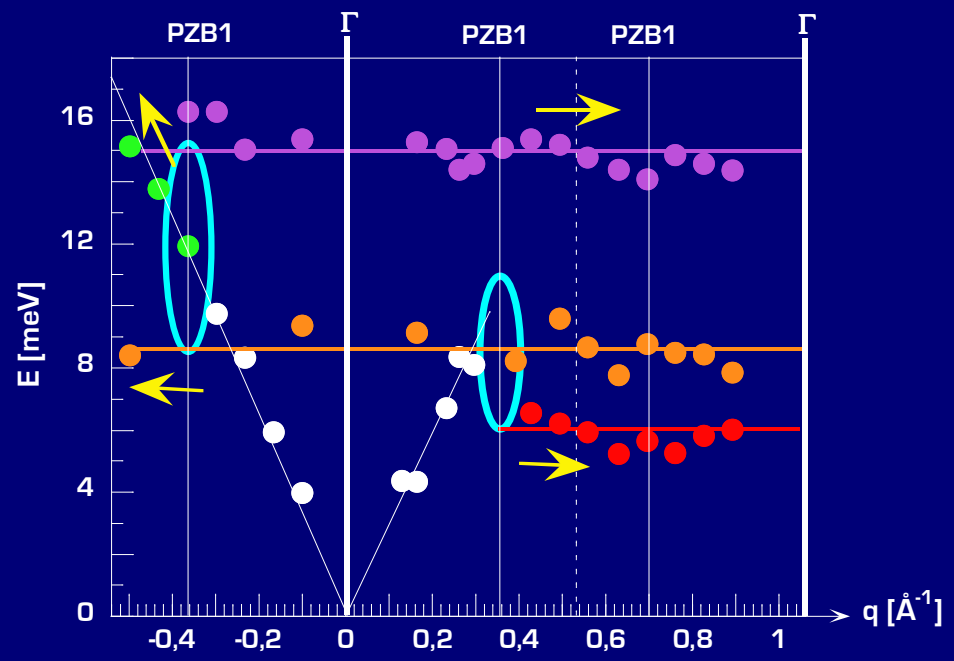
q ∈ [0, 0.33 Å^{-1}] :

Smooth evolution of the width

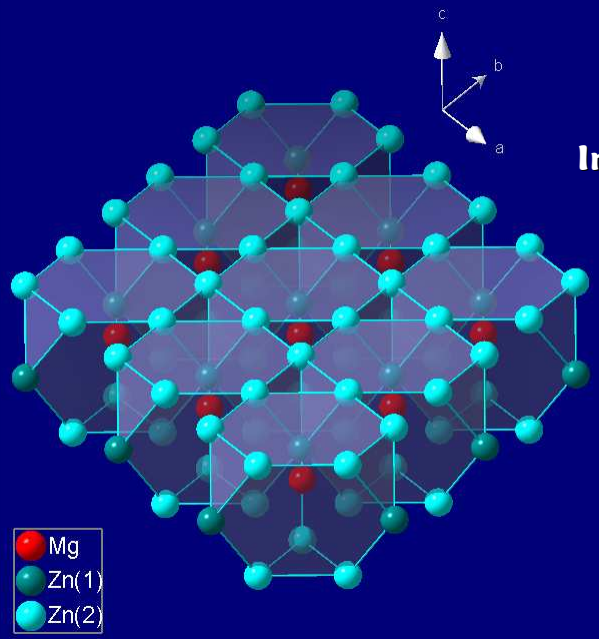
q ~ 0.36 Å^{-1} : strong broadening of the acoustic mode at the PZB1

q > 0.37 Å^{-1} : strong "modes mixing"

And spectral response dominated by the optic band at 15 meV



"Phonons" and phasons in QCs and related approximant phases



Lattice dynamics in a "simple phase" : the Zn_2Mg Laves Phase

Inelastic Neutron Scattering Measurements (IN8 and IN3@ILL, 2T1@LLB)

+ lattice dynamics simulation

Lattice dynamics in the i-$Cd_{5.7}Yb$ QC and its 1/1 Cd_6Yb approximant

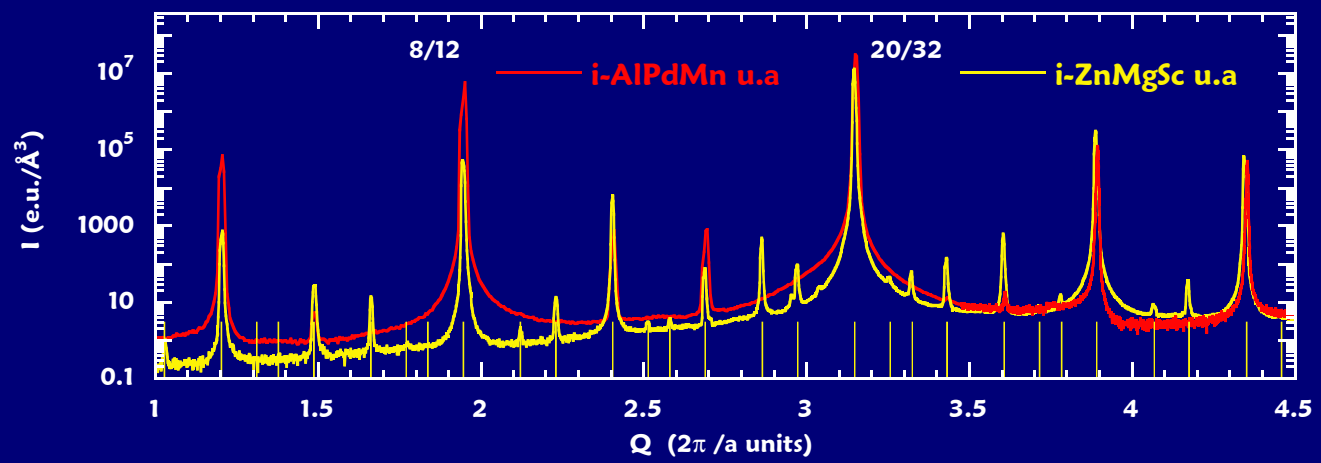
Inelastic X-ray Scattering Measurements (BL35XU@SPring-8)

Dynamics of Phason Fluctuations in the i-AlPdMn Quasicrystal

Coherent X-ray Measurements - IXFS (ID20@ESRF)

i-ZnMgSc QC and its 1/1 ZnSc approximant : Phonon Diffuse Scattering vs Phason Diffuse Scattering

X-ray Diffuse Scattering Measurements (D2AM/BM2@ESRF)



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