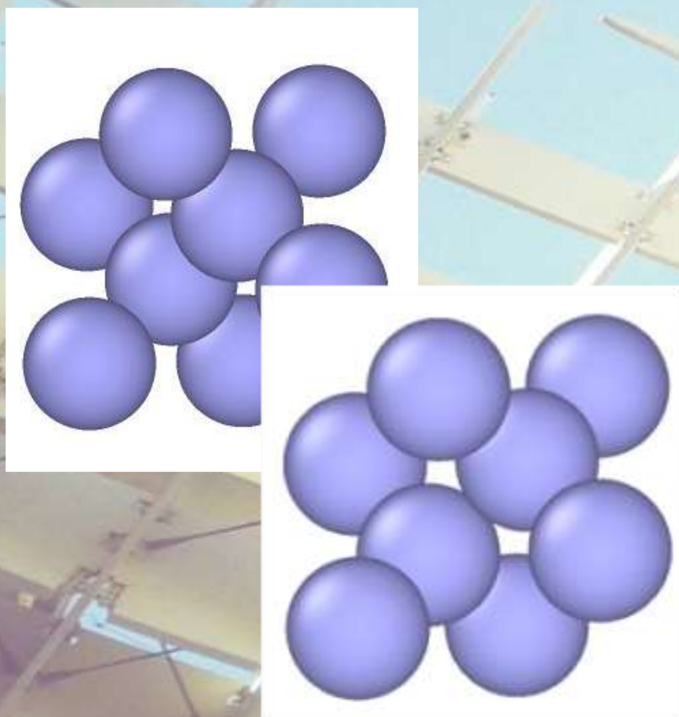
ON INTRINSIC LOCALIZED MODES, BREATHERS AND QUODONS

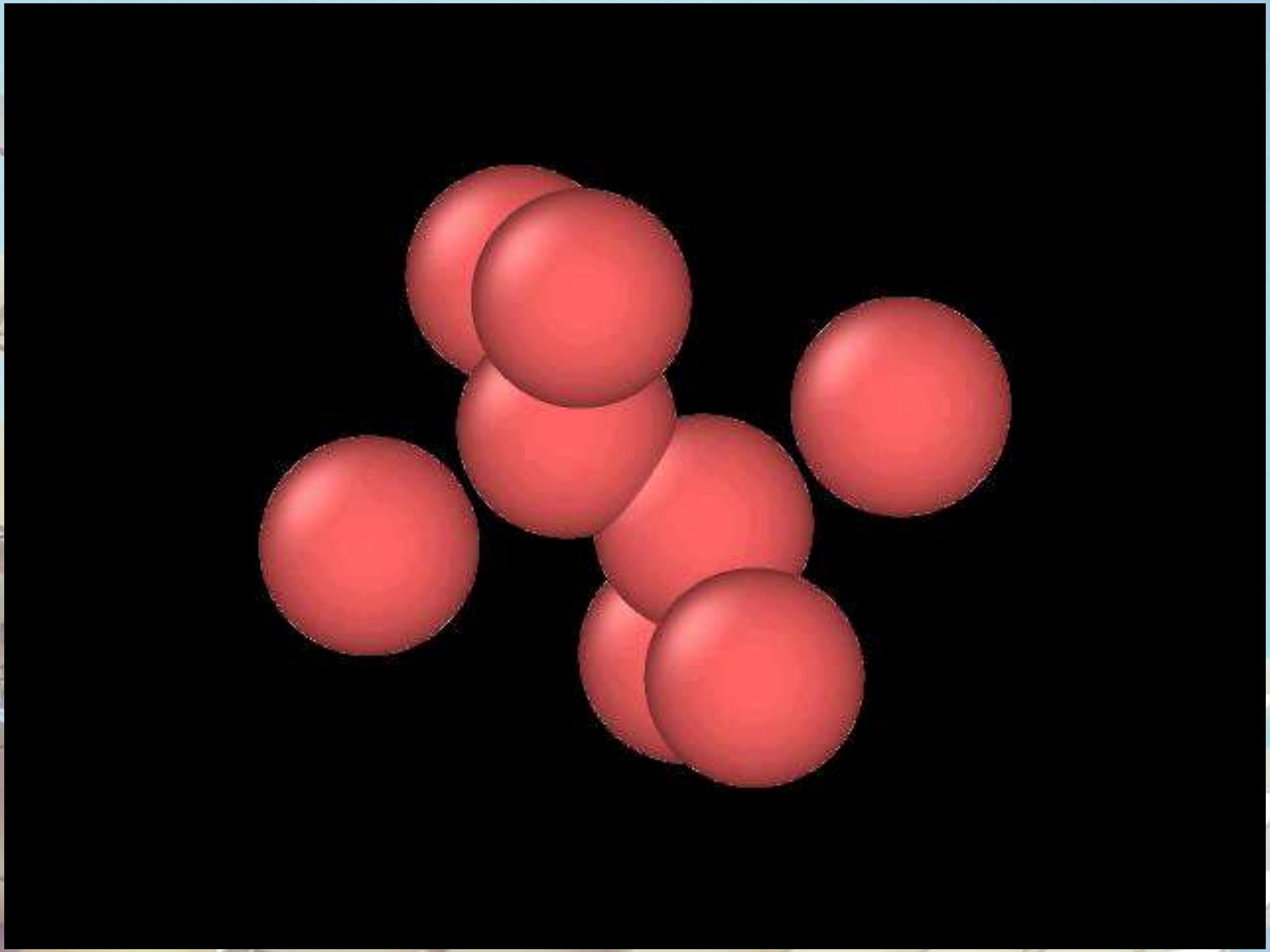
What are they?
Why do they exist?
Where do they exist?
Do they exist in crystals?
ILMs in germanium?
Quodons in mica muscovite?



Juan FR Archilla
Universidad de Sevilla
Spain

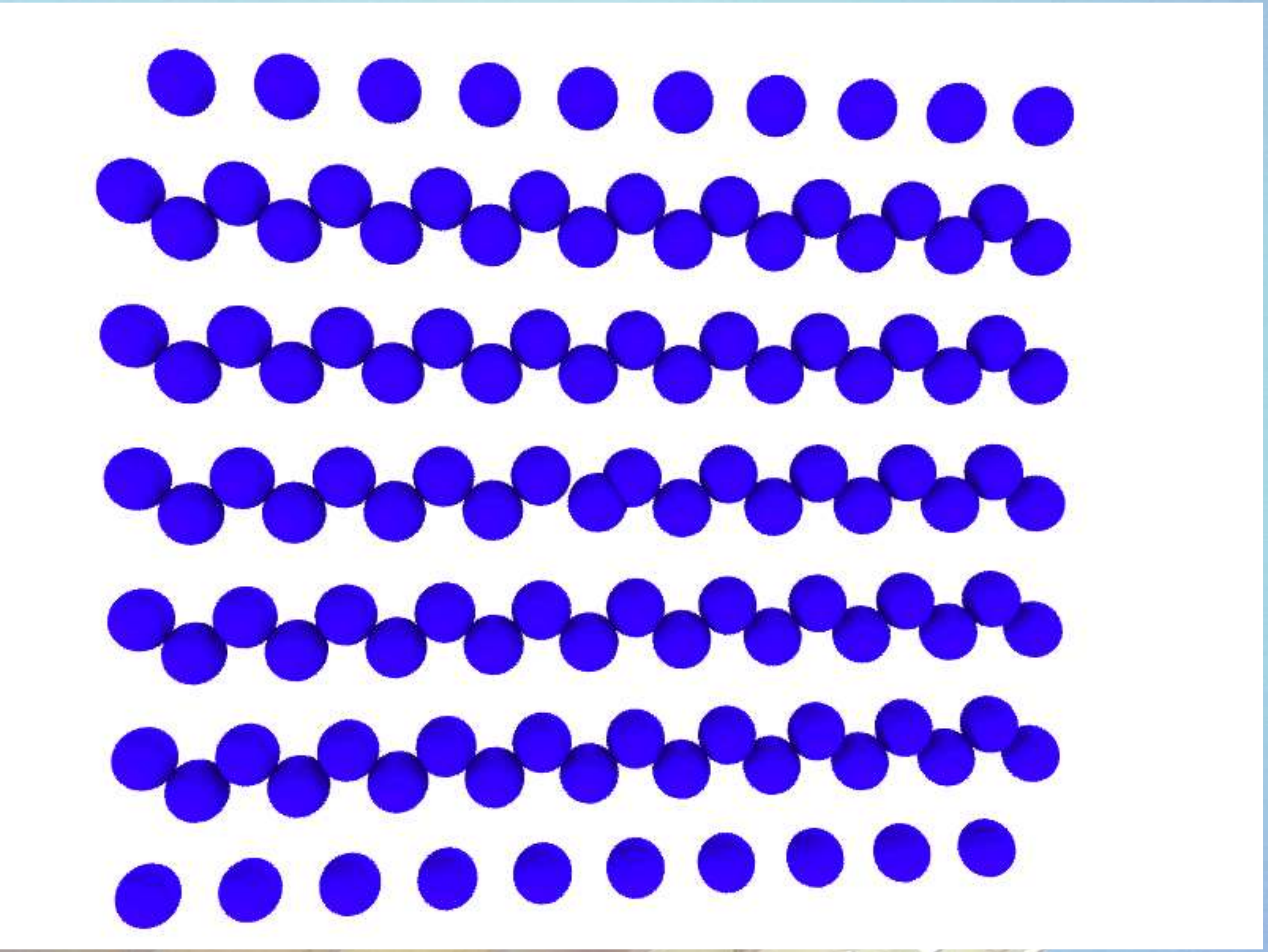
Helsinki, Accelerator Laboratory, Friday, June 12, 2015.

Discrete breather obtained with parcas MD code in Ge



Found by M. Klopov and V. Hizhnyakov using LAMMPS

Slice: discrete breather obtained with MD in Ge. F=1.25 THz



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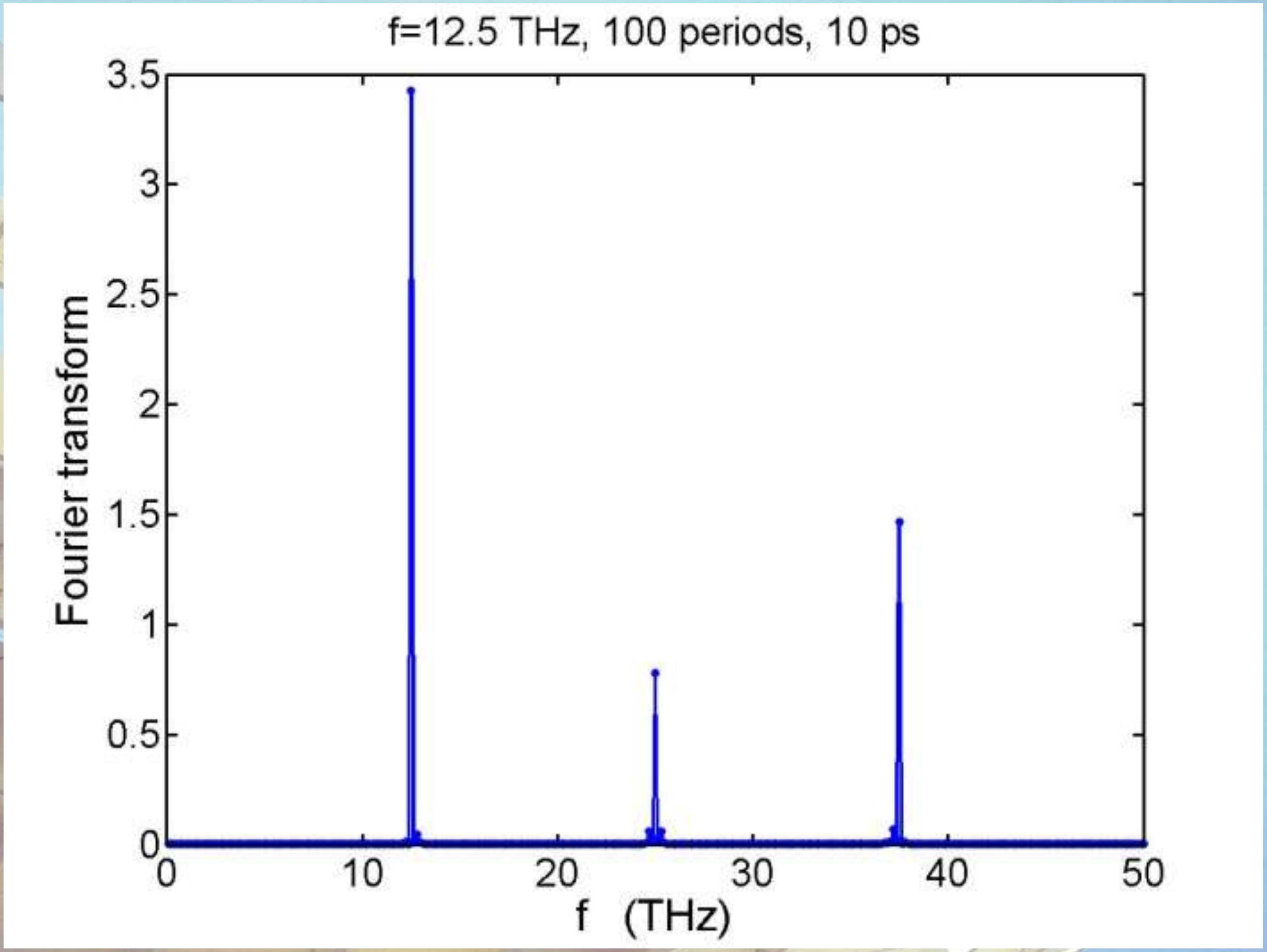
Fourier spectrum of the MD breather in Ge



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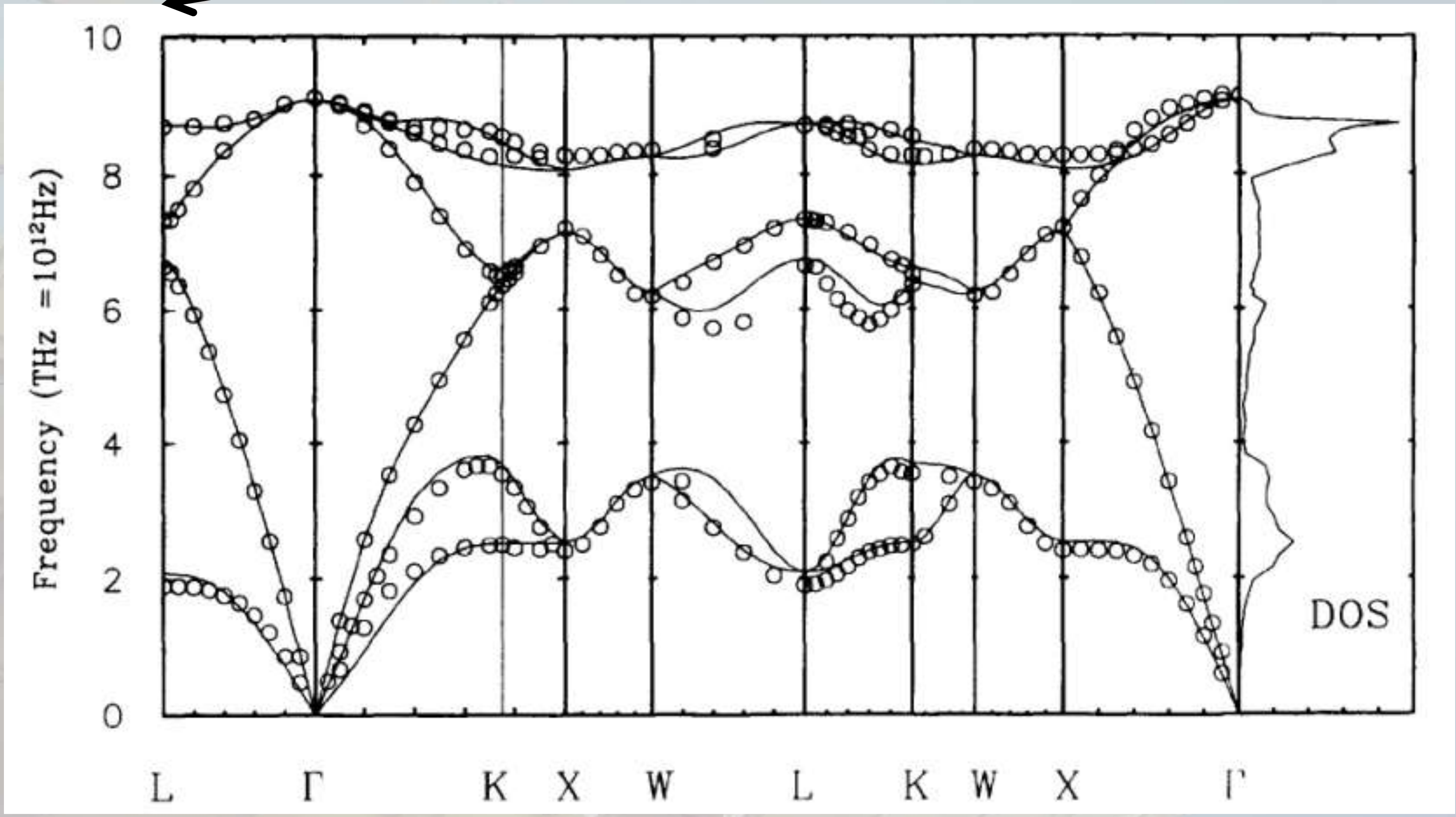
Density of states for germanium

Breather frequency in Ge



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So what is a discrete breather?

-Localized vibration in a periodic medium

-Two characteristics so far:

- -Localization
- -Nonlinear vibrations (some harmonics)
- -Well defined frequency outside the phonon spectrum

Many move

Typical energies: 0.5-5 eV

Are there other nonlinear intrinsic localized entities?

Yes:

-Solitons

-kinks

-Crowdions (replacement collisions cascade)

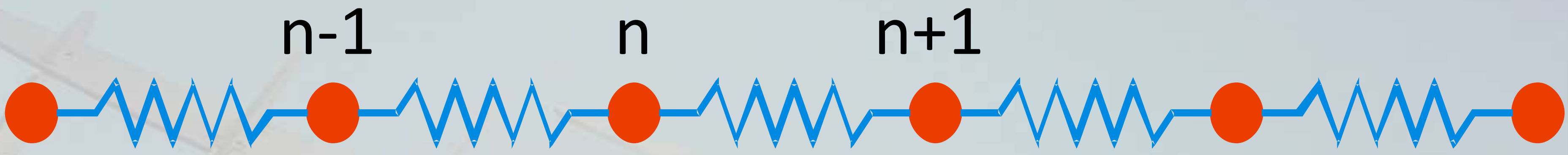
-Solelectrons and polarons

-Others: magnetic, spins

At least they exist in theory

İLMs for some is equal to breathers

Some basic maths



Suppose an 1D system: $$H=\sum_n \frac{1}{2}\dot{u}_n{}^2+\sum_n V(u_n)+\sum_n W(u)$$

Linearized: $$H=\sum_n \frac{1}{2}\dot{u}_n{}^2+\frac{1}{2}\sum_n \omega_0^2 u_n^2+\frac{1}{2}\sum_n \varepsilon(u_n-u_{n-1})^2$$

Dynamical equations: $$\ddot{u}_n=-\omega_0^2 u_n+\varepsilon(u_{n+1}+u_{n-1}-2u_n)$$

Trial solution $$u_n=A\mathrm{e}^{i(qn-\omega t)}$$

Solutions for frequencies $$\omega^2=\omega_0^2+4\varepsilon\sin^2(\frac{q}{2})$$

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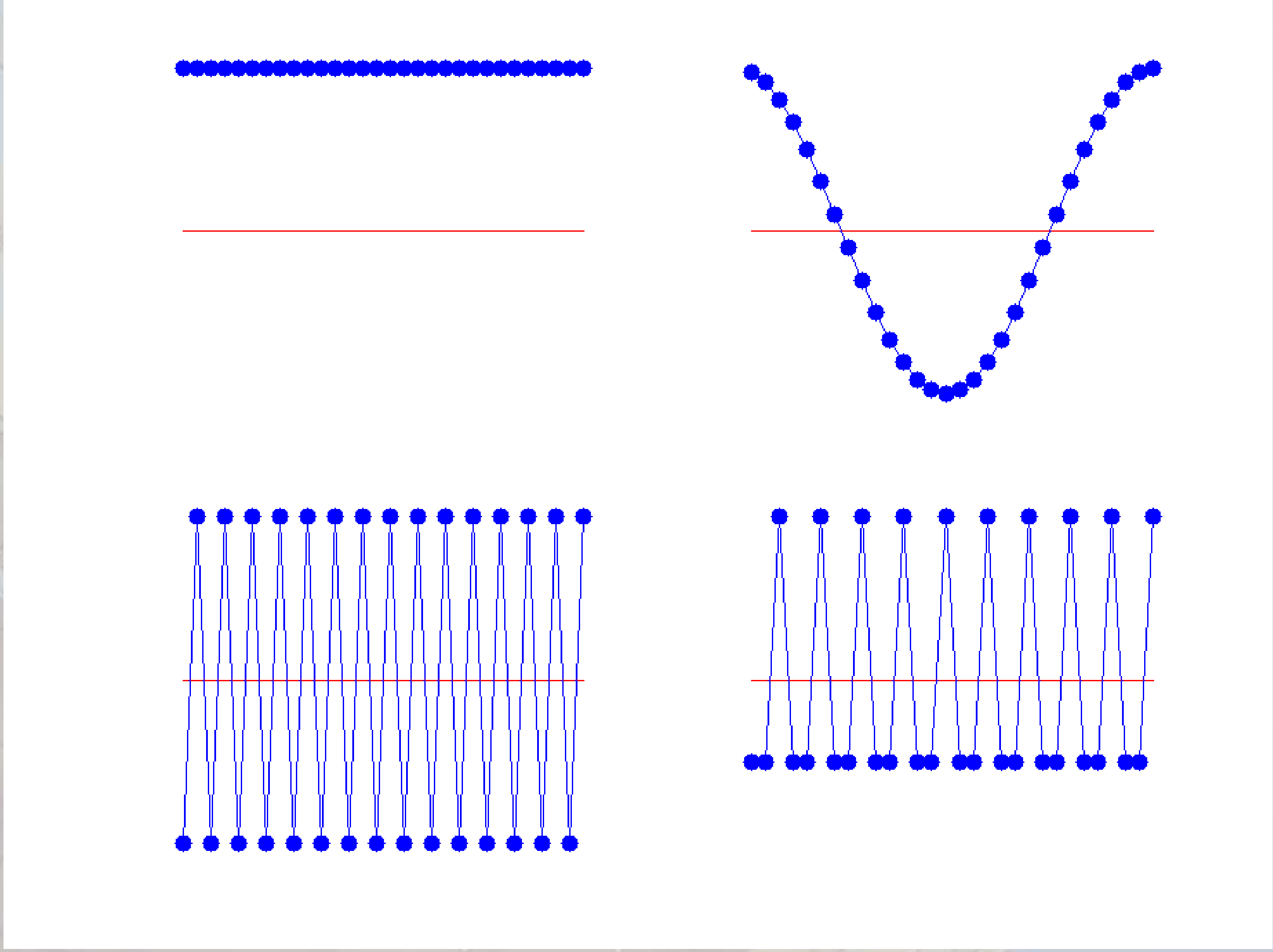
Phonons: $u_n = A\cos(q\,n - \omega_q t)$



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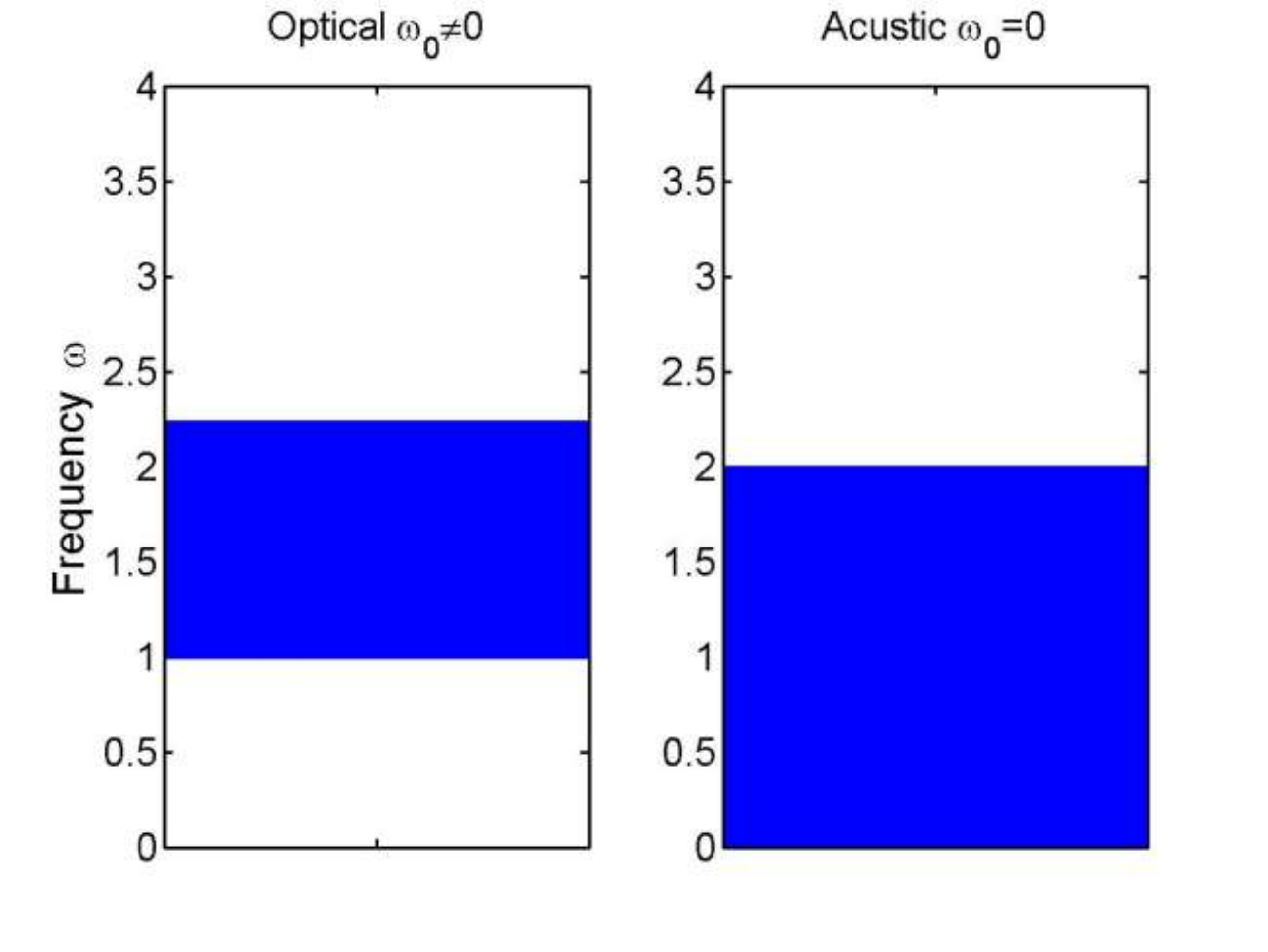
Phonon spectrum



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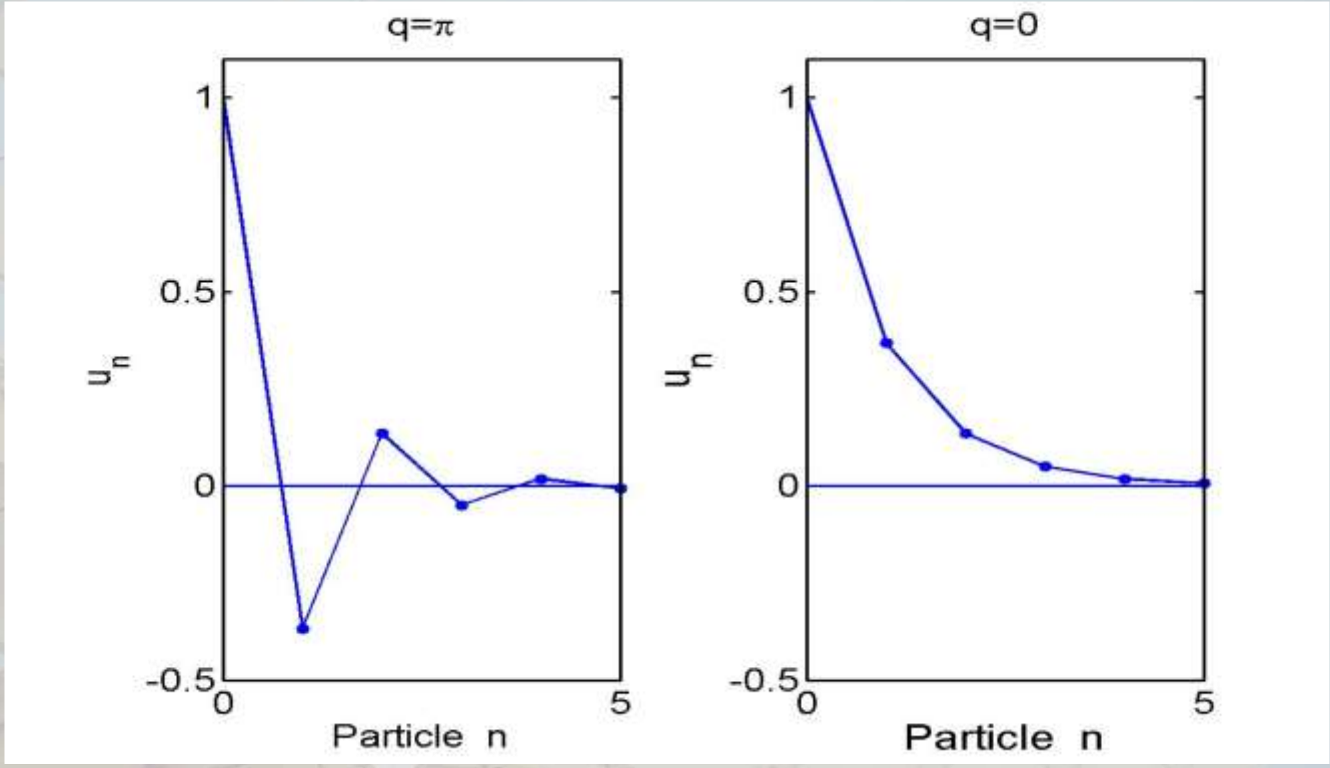
Trial solution for frequencies outside the phonon spectrum

$$u_n = A\mathrm{e}^{-\xi(n-Vt)}\mathrm{e}^{i(qn-\omega t)} \quad ; \quad n > Vt$$



$$\omega^2 = \xi^2 \mathrm{V}^2 + \omega_0^2 + 2\varepsilon(1 - \cos(\mathrm{q})\cosh(\xi))$$

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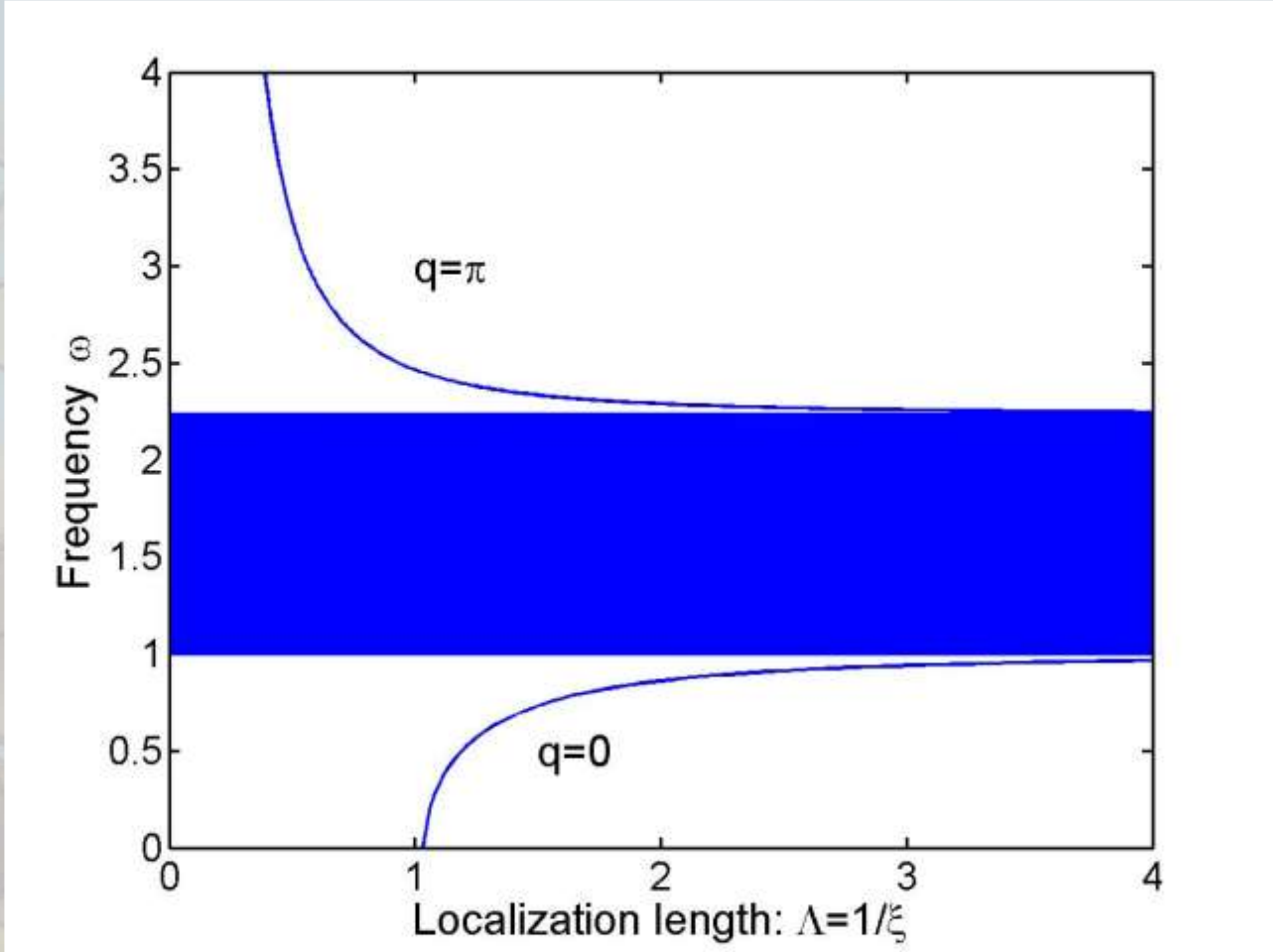
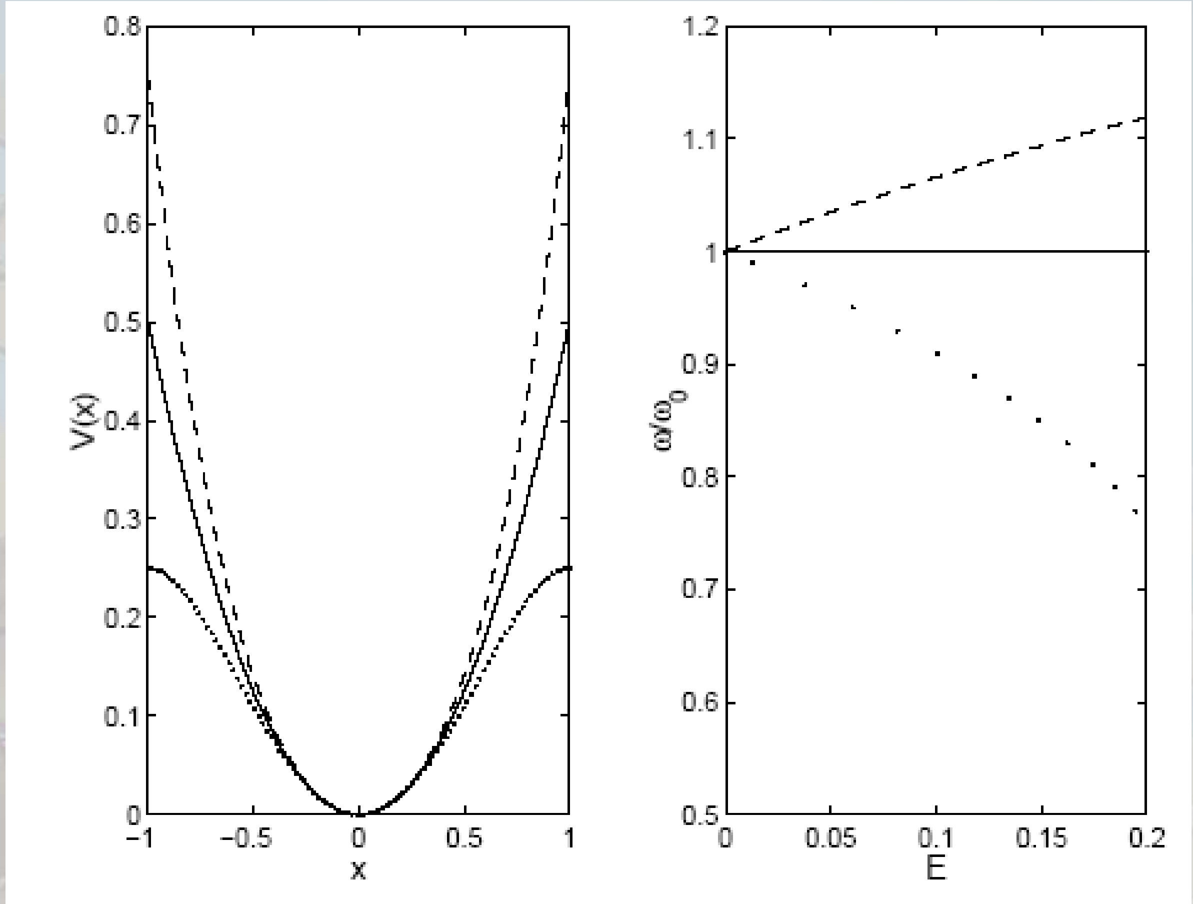
$$\omega\xi\mathrm{V} = \varepsilon \sin(\mathrm{q})\sinh(\xi)$$

Frequency versus localization length



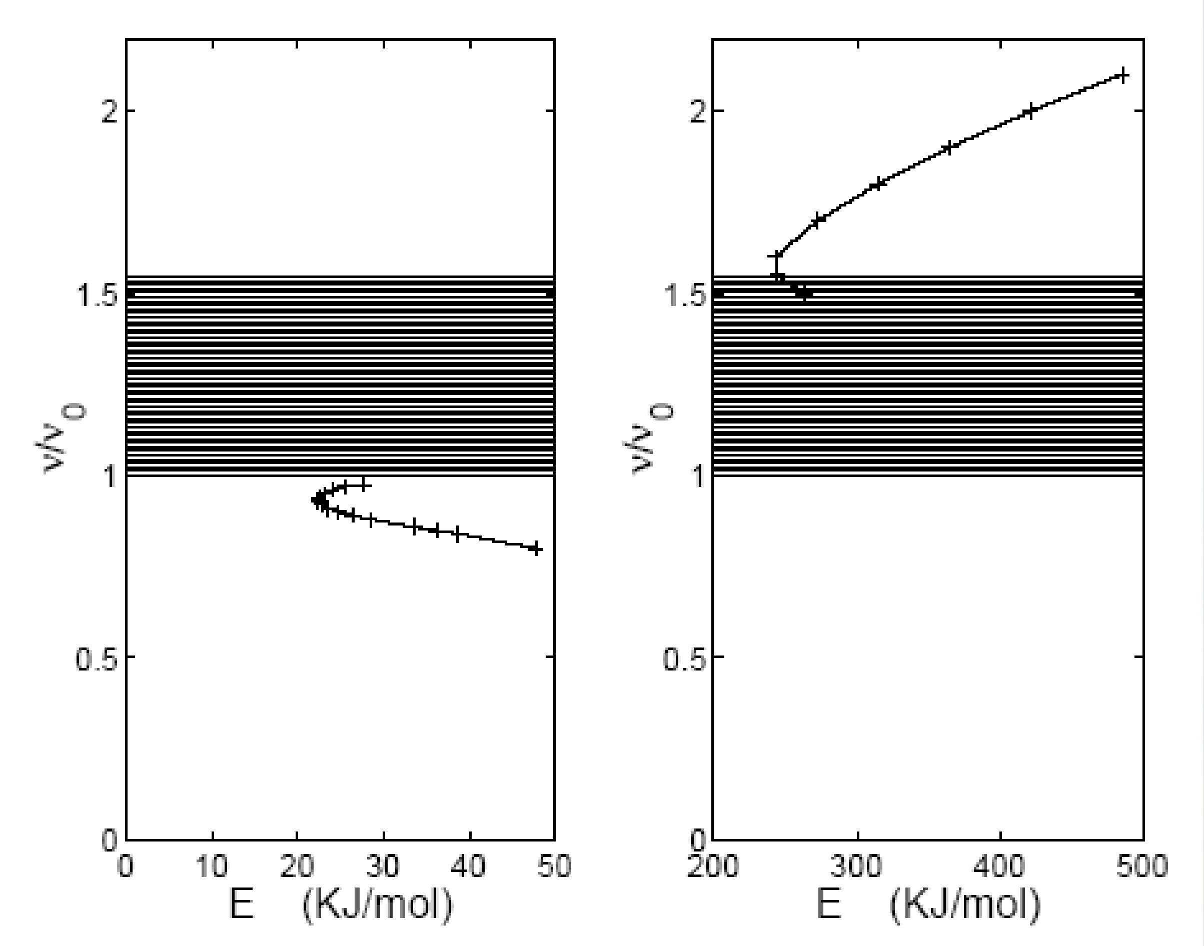
- The further apart from the phonon band, the more localization

Hard potential (--) / Soft potential (…)



Hard: frequency increases with amplitude/energy
Soft: frequency decreases with amplitude/energy

Hard breathers / Soft breathers



Sometimes we may have both in the same system:
As in ClNa structure

Necessary conditions for breather existence

Nonresonance: $n\omega_b \notin \text{phonon band}$

Nonlinearity: $\dfrac{\partial w_b}{\partial E} \neq 0$

Sufficient hardness if above the phonon band

In those conditions theorems stablish that breathers are exact solutions

So breathers exist in mathematical models, but do they exist in crystals?

In classical molecular dynamics

Ni, Nb,Fe, Cu, Ge, Si, NaCl, NaI, V,W, graphene, graphane, carbon nanotubes, C_{60},

With DFT in graphane, …

Some at finite temperature Fe 100K, Nb 300K,..

Not conclusive, but if they exist. Most likely:
They are not generic→ Few breathers, depending on the material and temperatures

In the real world?

By Mike Russell. It helped two persons to get jobs

Also in electrical lattices, arrays of Josephson junctions, cantilever arrays, waveguide arrays, …

In crystals:

Manley et al,   Uranium at 450-700K

Phys. Rev. Lett. 96, 125501 2006. Formation of a New Dynamical Mode in alpha-Uranium Observed by Inelastic X-Ray and Neutron Scattering

Physical Review B 77, 214305 2008 , Intrinsic nature of thermally activated dynamical modes in alpha-U: Non equilibrium mode creation by x-ray and neutron scattering

…….

In germanium?   Archilla, Coelho, Auret, Dubinko, Hizhnyakov (2015)

In mica muscovite?   Mike Russell, Eilbeck and coworkers since 1963

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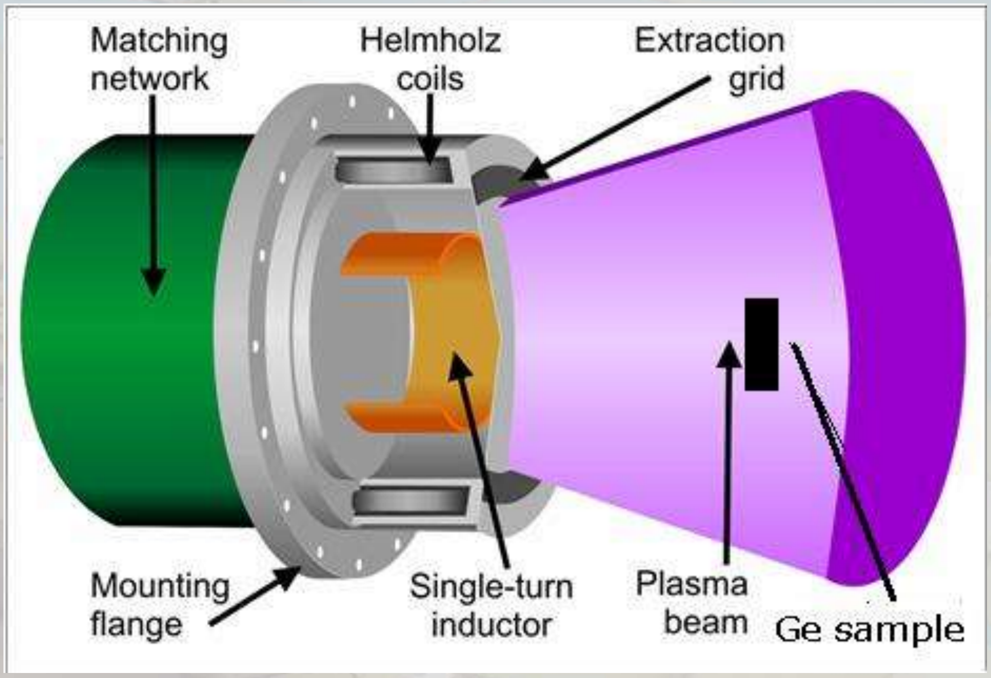
Plasma annealing of defects in germanium

Copra ICP Ar plasma source



Ge sample with an Au diode

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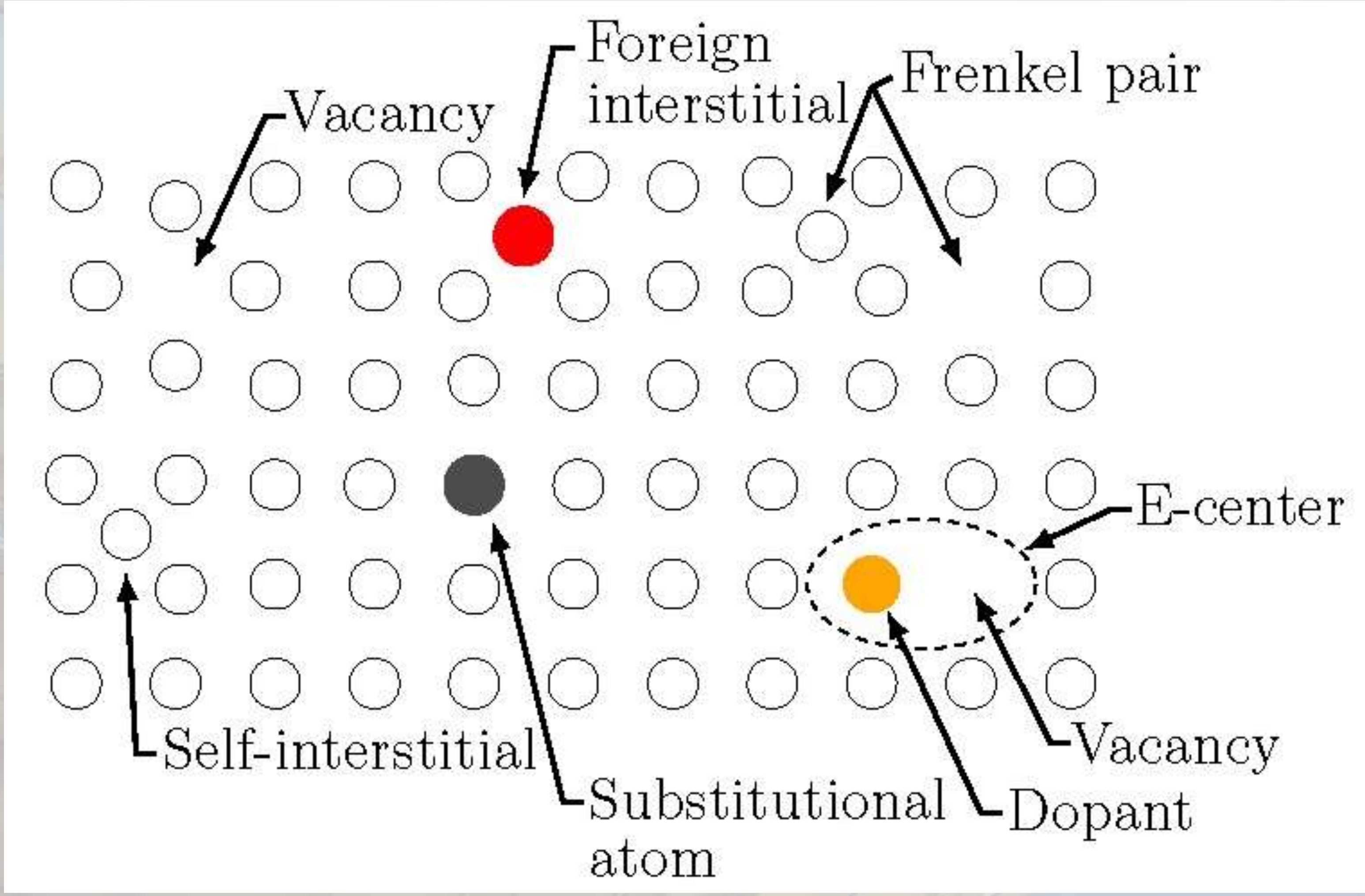
Sb-doped Ge

Defect detection by DLTS

N_{Ge}=4.42x10^{22} cm^{-3}
N_{Sb}=1.03x10^{15} cm^{-3}
N_{T}=1.07x10^{14} cm^{-3}

Defects in germanium

- Can be produced by irradiation
- Some vital, some fatal



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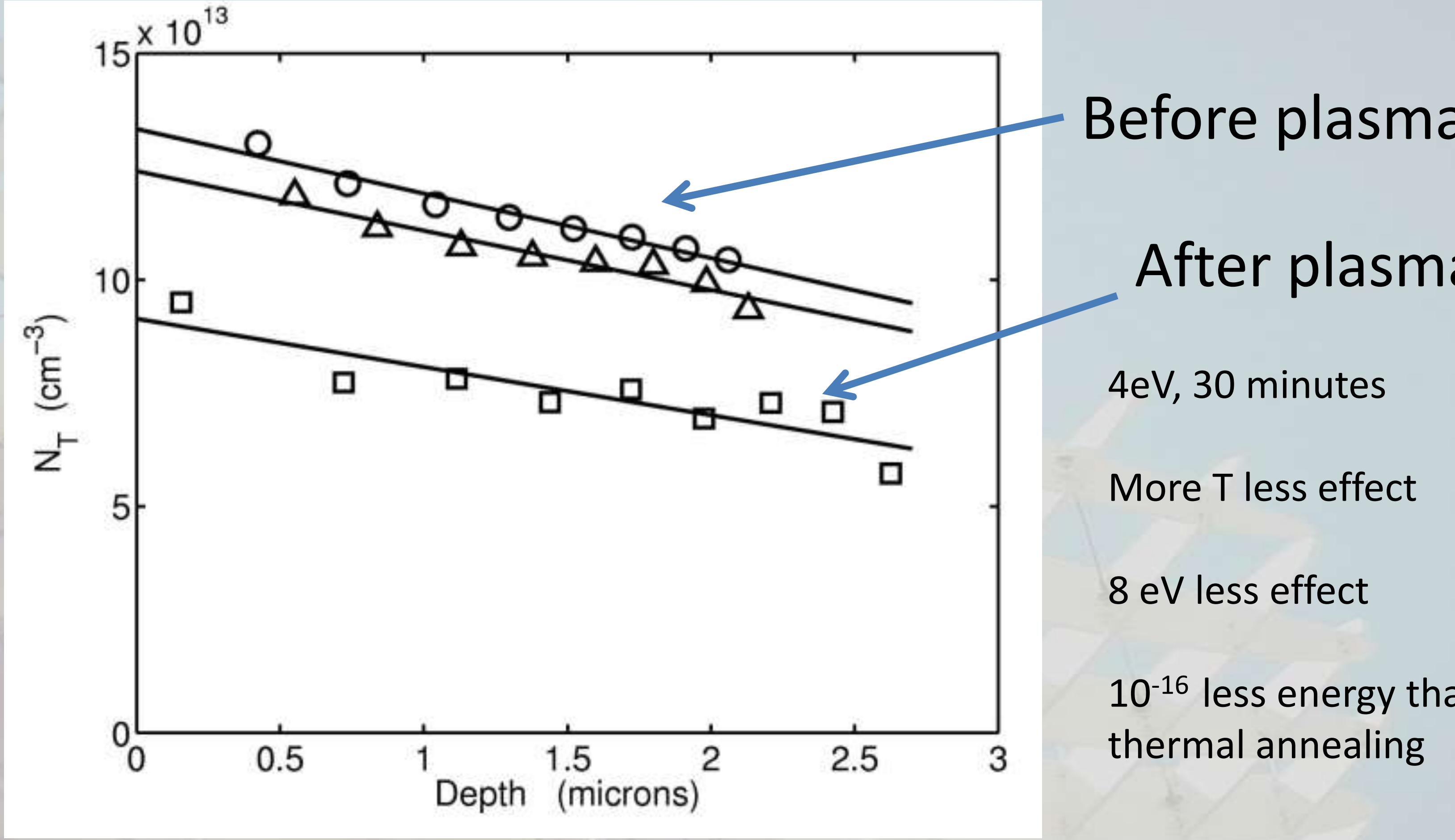
Concentration of E-center before and after plasma



4eV, 30 minutes

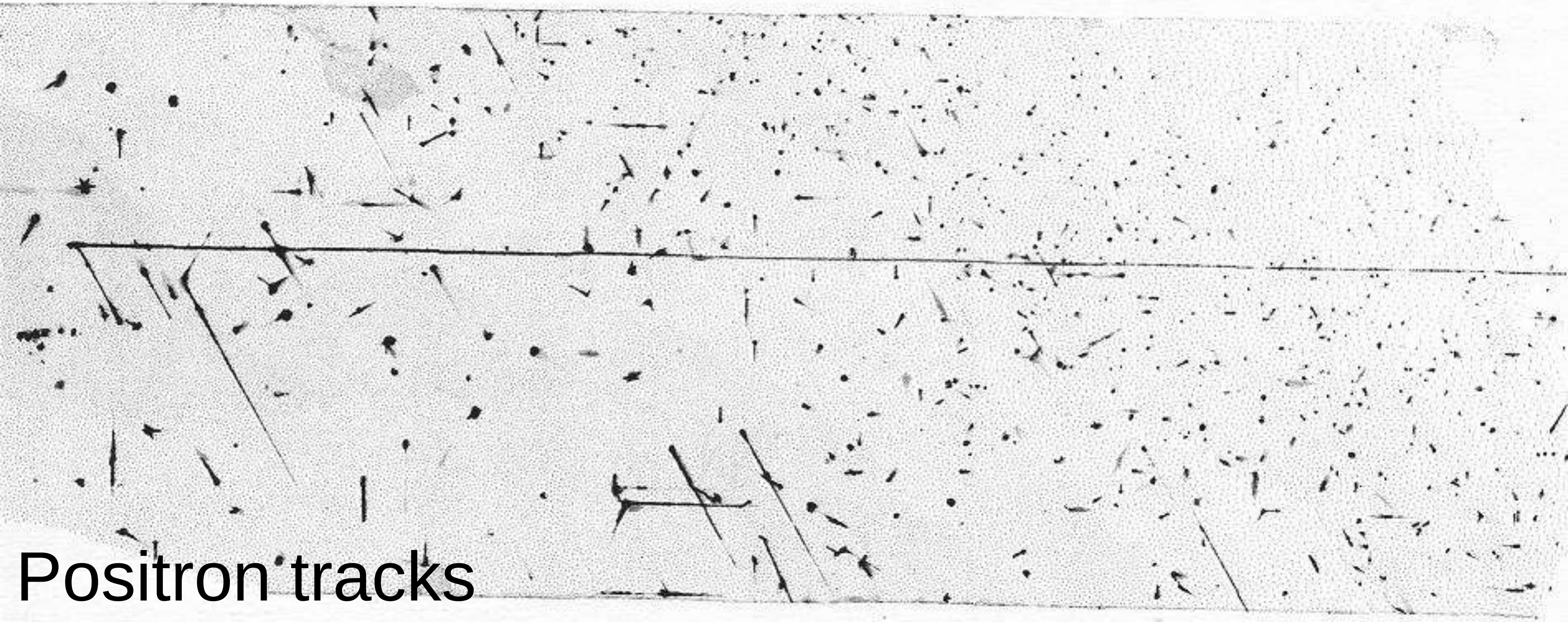
More T less effect

8 eV less effect

10^{-16} less energy than thermal annealing

. Archilla, J.F.R., Coelho, S.M.M., Auret, F.D., Dubinko, V.I., Hizhnyakov, V.: Long range annealing of defects in germanium by low energy plasma ions. Physica D 297, 56–61 (2015)

Quodons in mica muscovite



Positron tracks

- Produced in the decay of K^{40} with 0.5 MeV.
- 3 per second per cm^3
- Tracks are Fe oxides, magnetite

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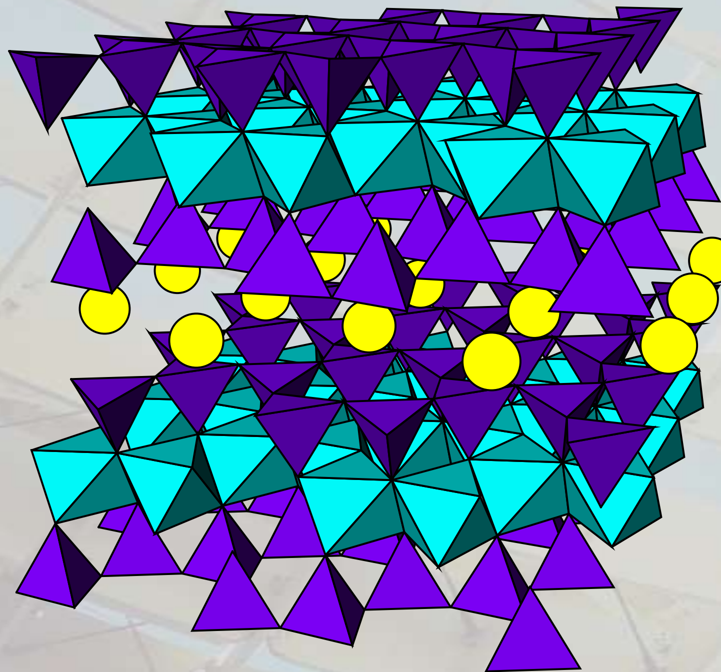
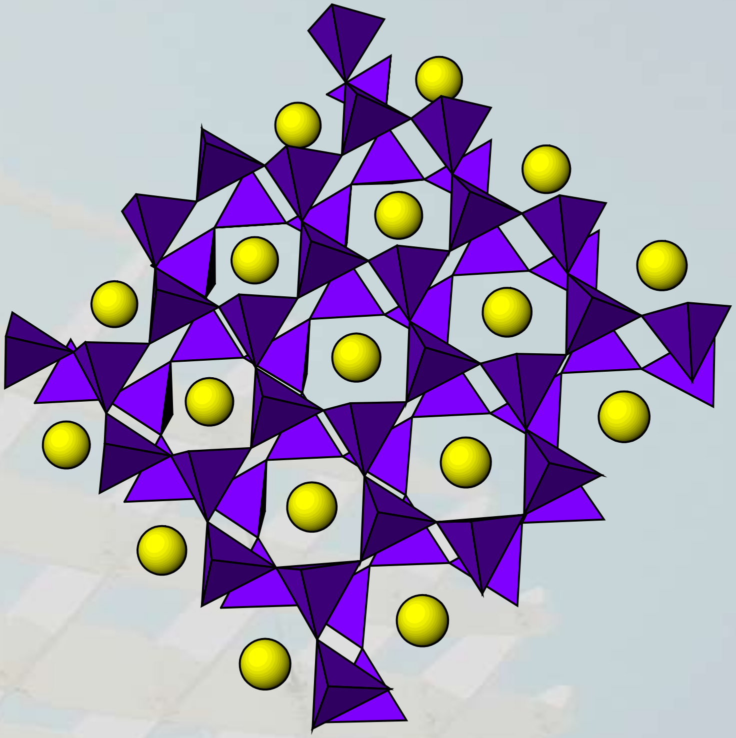
FM Russell, From Nature 1967, Nature 216, 907 ; 217 , 51 (1967) and many more

Mica muscovite. Cation layers

$K_2[Si_6Al_2]^{IV}[Al_4]^{VI}O_{20}(OH)_4$

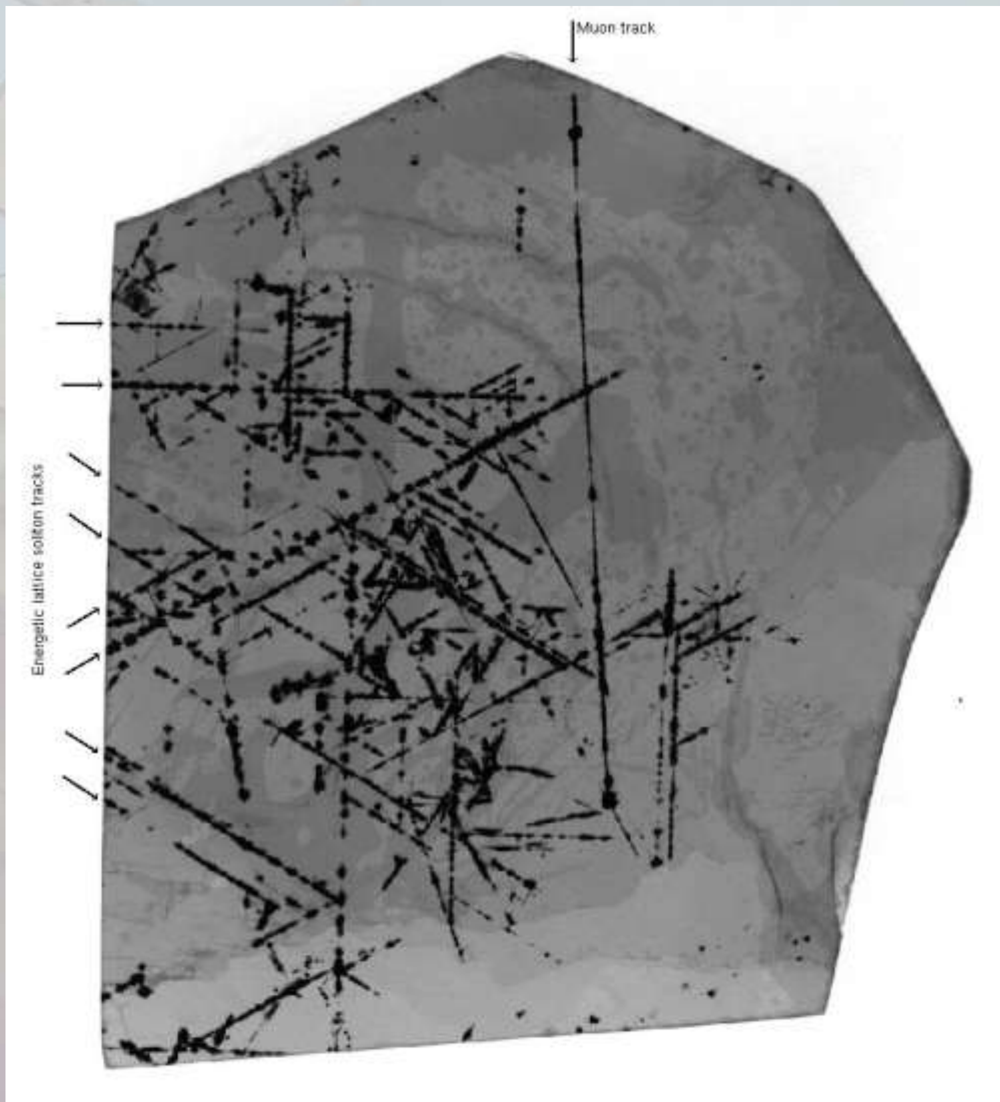




K^+ : 2D lattice of repulsive particles

K^+

Quodons: quasi one-dimensional excitations of the lattice in mica muscovite



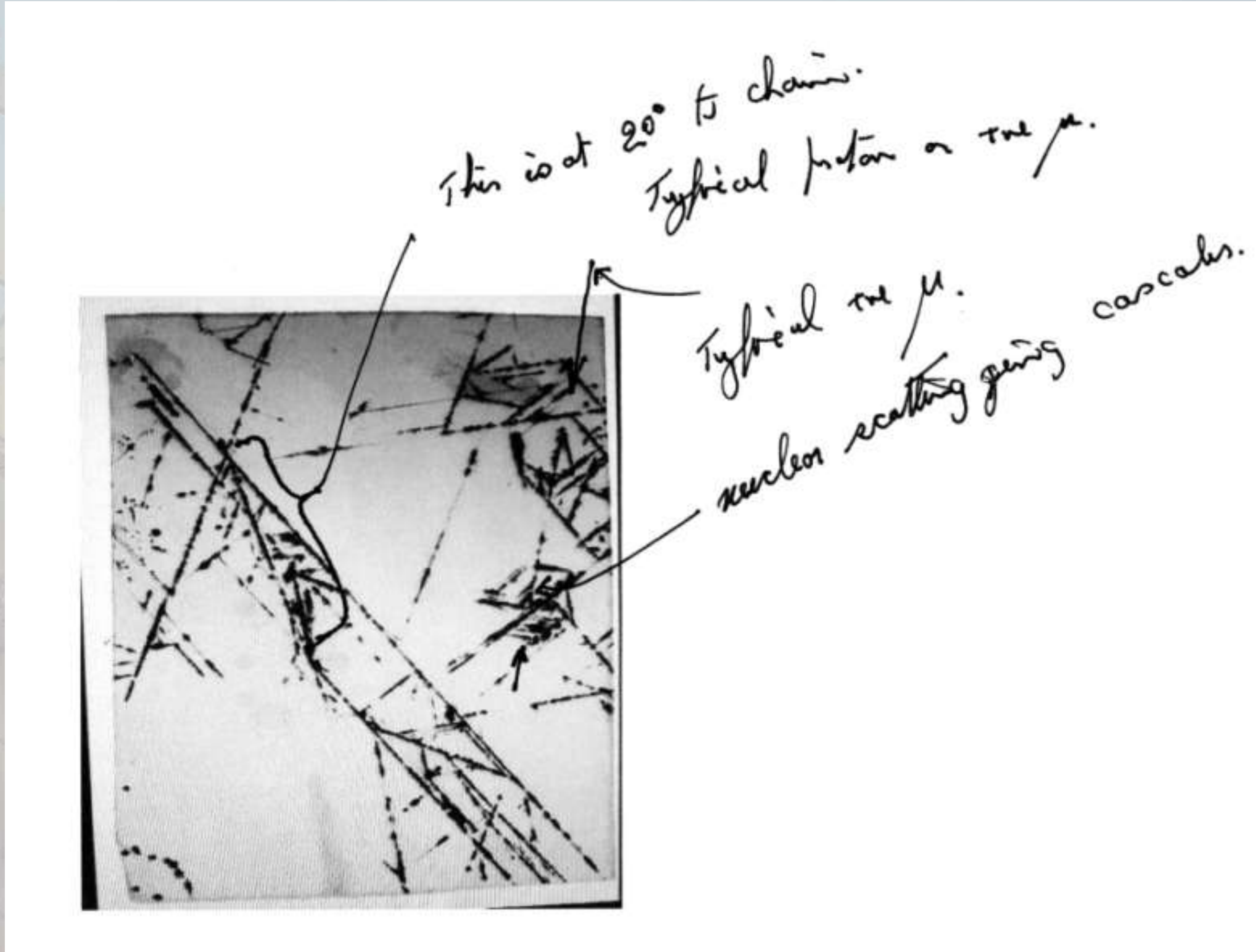
Tracks: magnetite Fe_3O_4

Causes

- 0.1% Swift particles
    - muons: after neutrino interaction
    - Positrons: decay of 40K
- 99.9% unknown: most in lattice close packed directions

Anharmonic lattice vibrations?

The piece of mica in your hands



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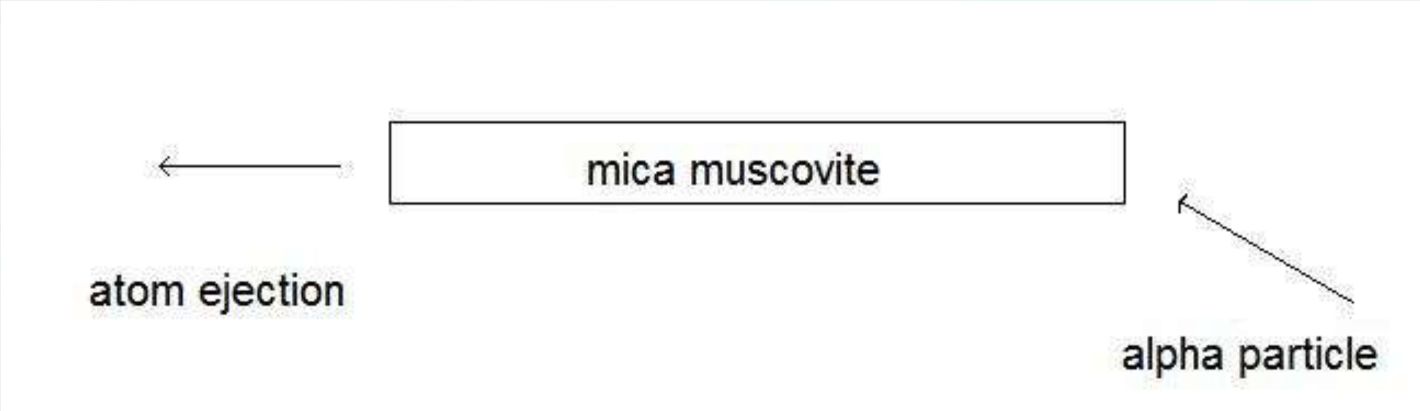
Experimental evidence of travelling excitations in mica muscovite



Trajectories were along lattice directions within the K^+ layer .
Surface binding energy of ejected atoms unknown:
typical values 3-8 eV

Russell, F.M., Eilbeck, J.C. (2007). Evidence for moving breathers in a layered crystal insulator at 300K. *Europhysics Letters* 78, 1004, 1-5.

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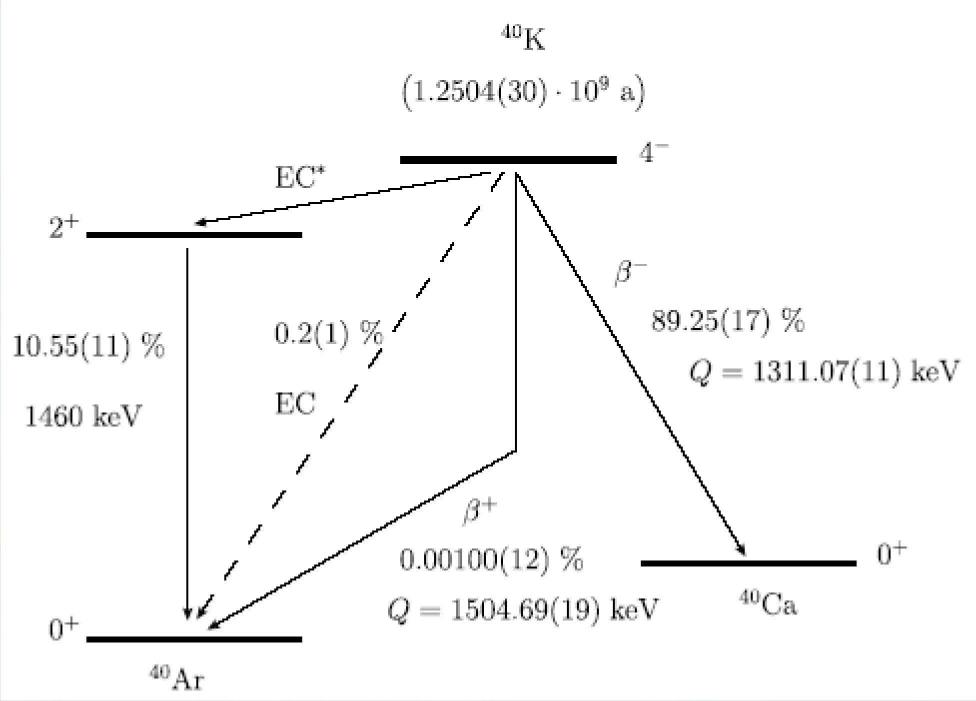
What about charge?

Almost all the decay modes of ^{40}K leave a charge behind,



A supersonic crowdion in mica, Archilla et al, in Quodons in Mica, Archilla et al, Eds, Springer (2015)

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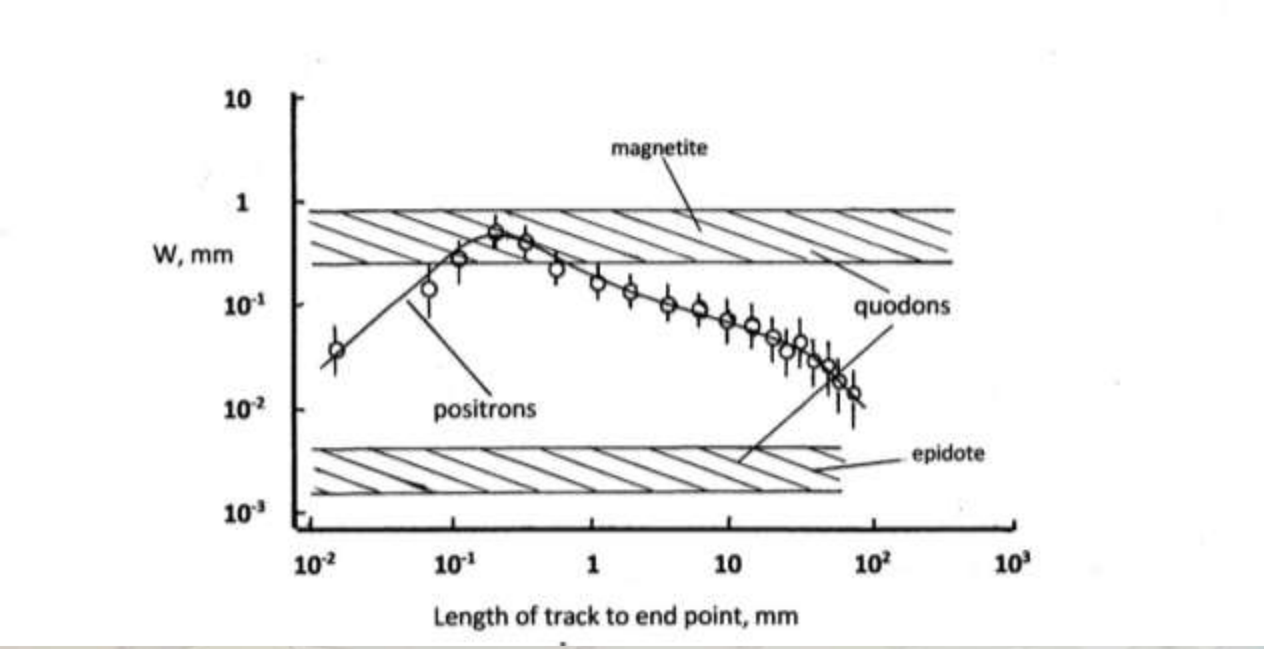
Table 2 Table of decays for ^{40}K

Decay	β^-	EC1	EC1+CE[1]	EC2[2]	β^+
Intensity	89.25%	10.55%	0.001%	0.2%	0.001%
T (keV)	1311.07	1460	1460	1504.69	483.7
Emitted charged particle	e^-		e^-	e^-	e^+
Recoil from	ν+e^-	γ	e^-	ν	ν+e^+
Max Recoil (eV)	42	29.2^M	49.7^M	31.1^M	10
Daugther ion (A=40)	Ca^{++}	Ar^+	Ar^{++}	Ar^{++}	Ar
Max V (Km/s)	14.4	12^M	15.7^M	12.2^M	7
Ionization of daughter (eV)	50.6	27.7	40.8	40.8	15.8
Δq (e)	+1	0	+1	+1	-1

[1] Subset of EC1 when the gamma is delivered to a shell electron; ^{M} Monocromatic
[2] Direct decay to Ar ground state, recoil from neutrino emission; 3 KeV Auger e^-
EC: electron capture; CE: conversion electron; T: energy available excluding rest masses
Ionization energy of K^+ 31.6 eV

Quodons may have charge (2015)

-90% of the decay modes leave a **positive** charge behind (beta – decay)
- Only positive swift particles leave tracks
- Positrons at near sonic speed leave the same tracks than quodons



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FM Russell (2015), arXiv:1505.03185

Many thanks for your attention

Archilla, Russell and Coelho, Altea, Spain, 2013
Conference: Quodons in mica: nonlinear localized travelling excitations in crystals.
To appear, Springer 2015

Many thanks for your attention

Archilla, Hizhnyakov and Dubinko, Tartu, Estonia, November 2012
Workshop: Lattice solitons and irradiation-induced nonlinear phenomena in solids,

Some bibliography

Long range annealing of defects in germanium by low energy plasma ions
JFR Archilla, SMM Coelho, FD Auret, VI Dubinko and V Hizhyakov
Physica D 297 (2015) 56-61

Ultra-discrete kinks with supersonic speed in a layered crystal with realistic potentials,
JFR Archilla, Yu A Kosevich, N Jiménez, V Sánchez-Morcillo and LM García-Raffi
Phys. Rev. E 91 (2015) 022912

Reaction rate theory with account of the crystal anharmonicity
VI Dubinko, P.A. Selyshchev and JFR Archilla,
Phys Rev E 83 (2011) 041124

Discrete breathers for understanding reconstructive mineral processes at low temperatures
JFR Archilla, J Cuevas, MD Alba, M Naranjo and JM Trillo ,
J. Phys. Chem. B 110 (2006) 24112

Haas, M., Hizhnyakov, V., Shelkan, A., Klopov, M., Sievers, A.J.: Prediction of highfrequency intrinsic localized modes in Ni and Nb.
Phys. Rev. B **84, 144,303(1–8) (2011)**