UNIVERSITAT POLITÈCNICA DE VALÈNCIA
UNIVERSIDAD DE SEVILLA
IGIC Instituto de Investigación para la Gestión Integrada de Zonas Costeras
IUMPA

Quodons in Mica 2013 /// Meeting in honour of Prof. Mike Russell.

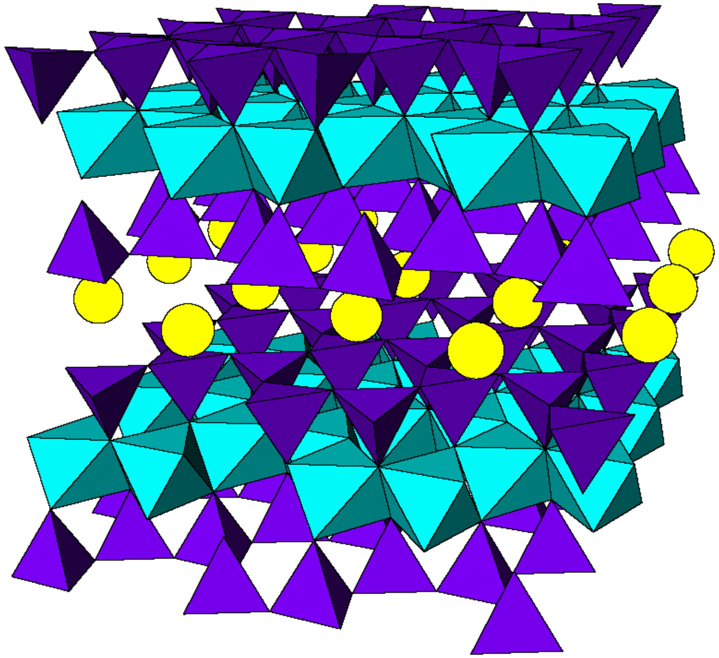
A crowdion in mica

Between K^{40} recoil and transmission sputtering

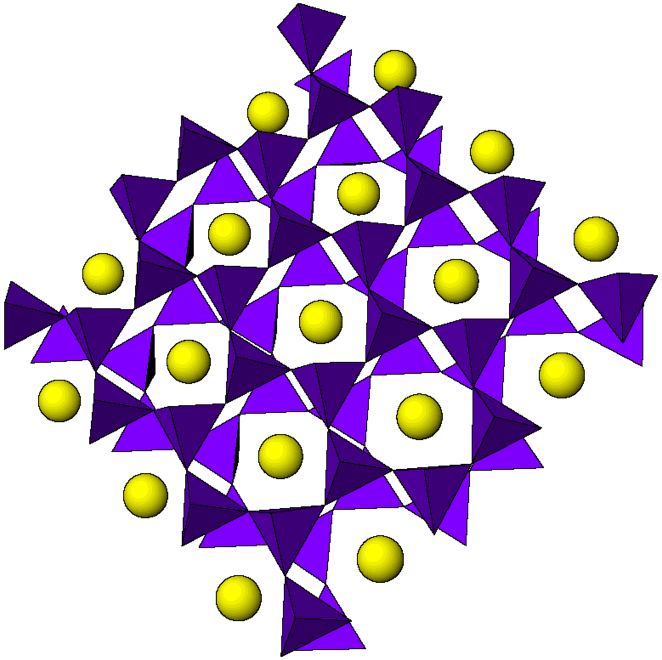
Noé Jiménez /// Juan FR Archilla /// Yuriy Kosevich,
Víctor Sánchez-Morcillo /// Luis Miguel García-Raffi

Motivation: The mica

- Stratified silicate



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

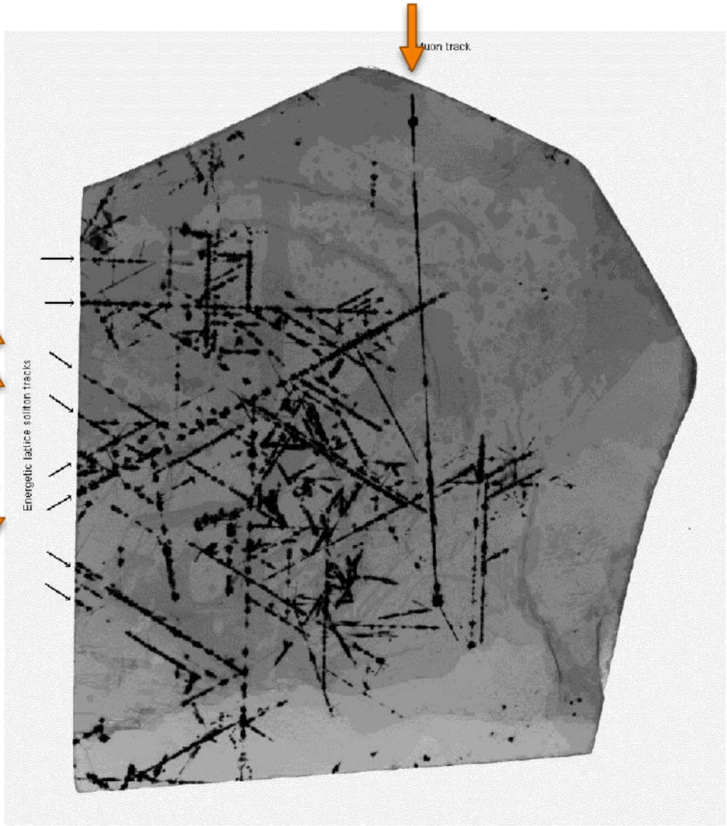


● K^+

Tracks recorded by mica

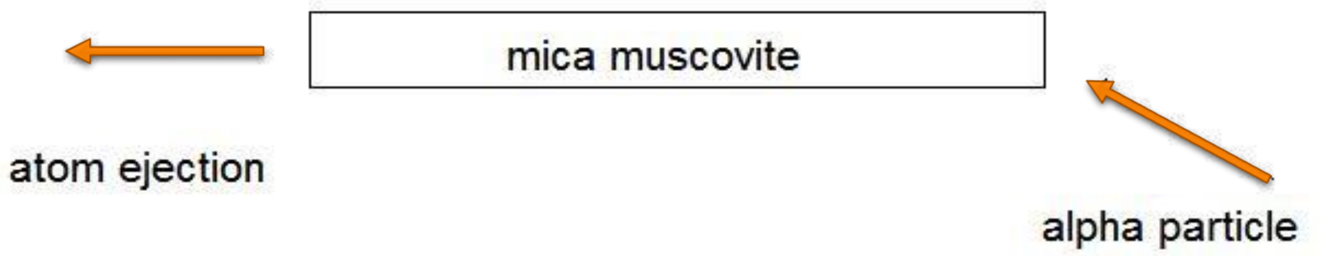
- 0.1% of the tracks are explained because of charged particles, like muons, positrons, electron cascades.
- 99.9% of the tracks are within the lattice closed packed lines in the (001) plane.

Quodons:
quasi one-dimensional excitations



D.R. Collins et all, *Phys. Chem. Minerals*. 19: 520-527 (1993)
G. Brudeylins, D. Schmicker,. *Surface Science*, 333: 237-242 (1995)
Schlößer, D., Russell, F.M. et. all. Radiation Measurements 23, 209-213. (1994)

Experimental evidence of travelling excitations in mica muscovite

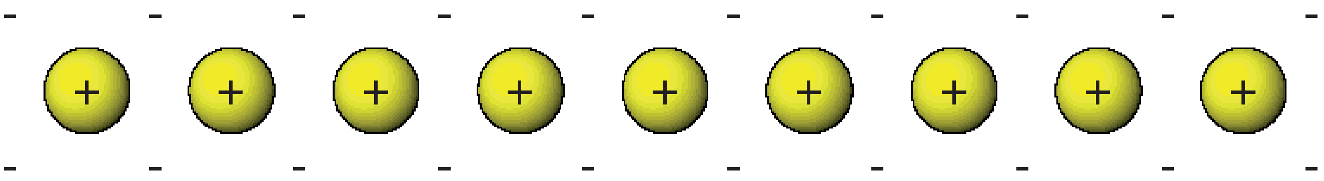


Russell, F.M., Eilbeck, J.C. (2007). Evidence for moving breathers in a layered crystal insulator at 300K. Europhysics Letters 78, 1004, 1-5.

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

Minimal model of a Coulomb repulsive lattice

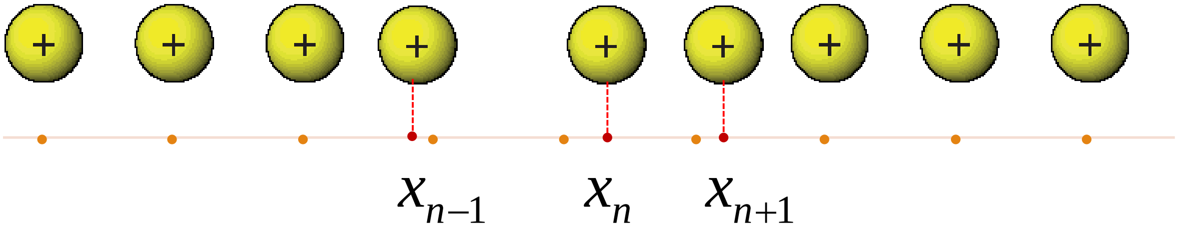
- Coulomb 1D Repulsive lattice



- Longitudinal perturbations
- Coulomb’s repulsion is rapidly screened
- We limit initially to nearest neighbors (N= 1 - 6)
- Negative charge at the borders keep cations inside

Minimal Model

- Displacements



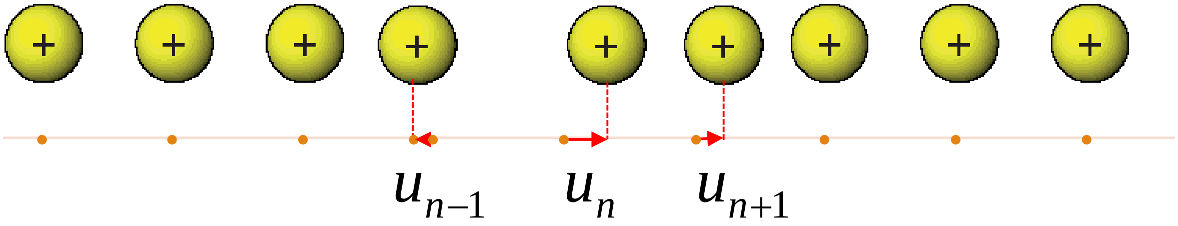
- Movement equation

$$m_k \frac{\partial^2 x_n}{\partial t^2} = -\frac{Ke^2}{\left(x_{n+1} - x_n\right)^2} + \frac{Ke^2}{\left(x_n - x_{n-1}\right)^2}$$

Minimal Model

- Normalization

Speed 2.6 km/s; Energy 2.8 eV; frequency 5 THz



- Movement equation

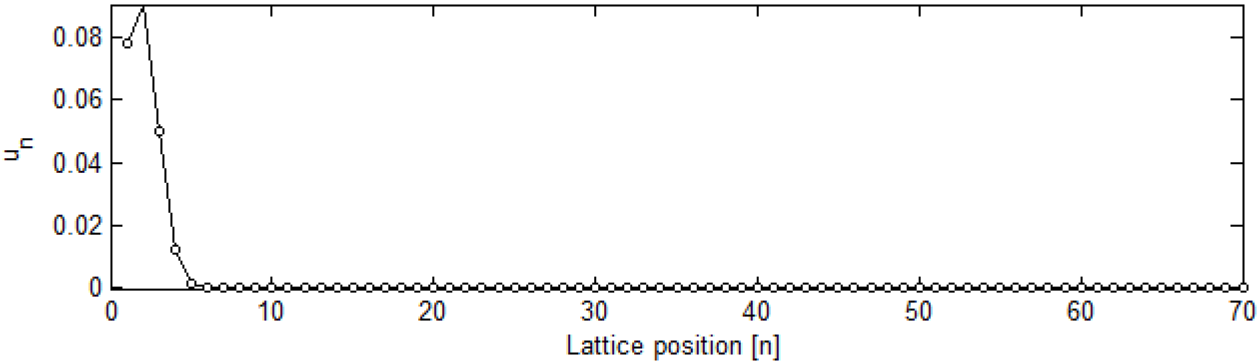
$$\frac{\partial^2 u_n}{\partial t^2} = -\frac{1}{\left(1+u_{n+1}-u_n\right)^2} + \frac{1}{\left(1+u_n-u_{n-1}\right)^2}$$

$$v_n = u_n - u_{n-1}$$

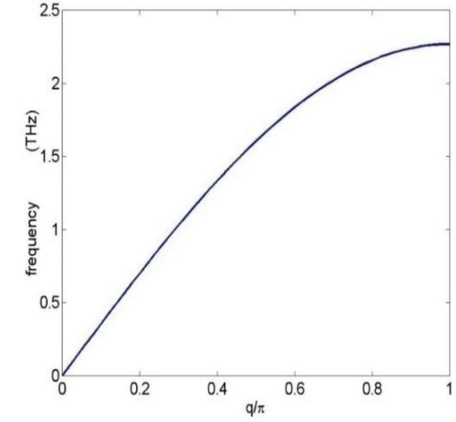
Small amplitude perturbation

$$u_{n=1}(t) = A_0 \sin(\omega t) \qquad \text{for} \qquad \omega t < \pi$$

- $A_0 = 0.09$

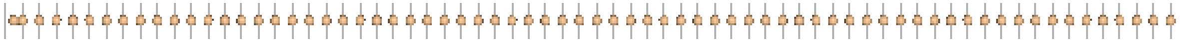


- Phonon velocity spectrum

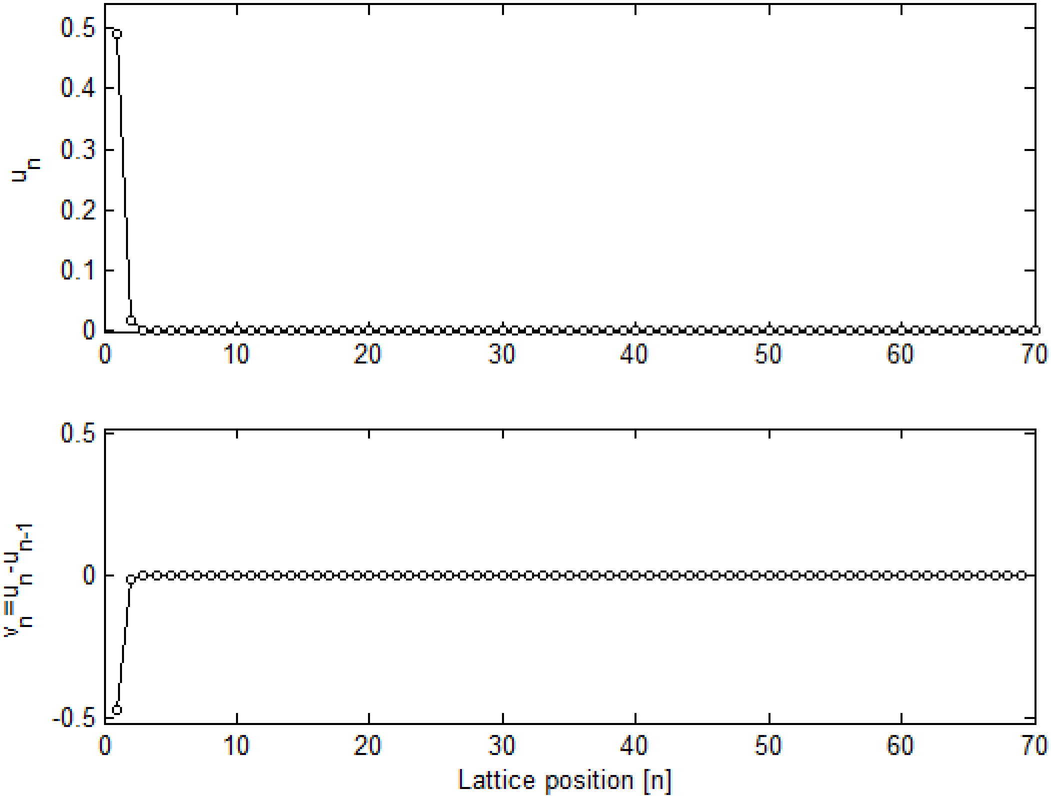


Kink N=1

$$u_{n=1}(t) = A_0 \sin(\omega t) \quad \text{for} \qquad \omega t < \pi$$



$$A_0 = 0.95$$



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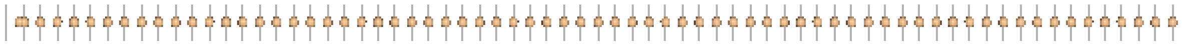
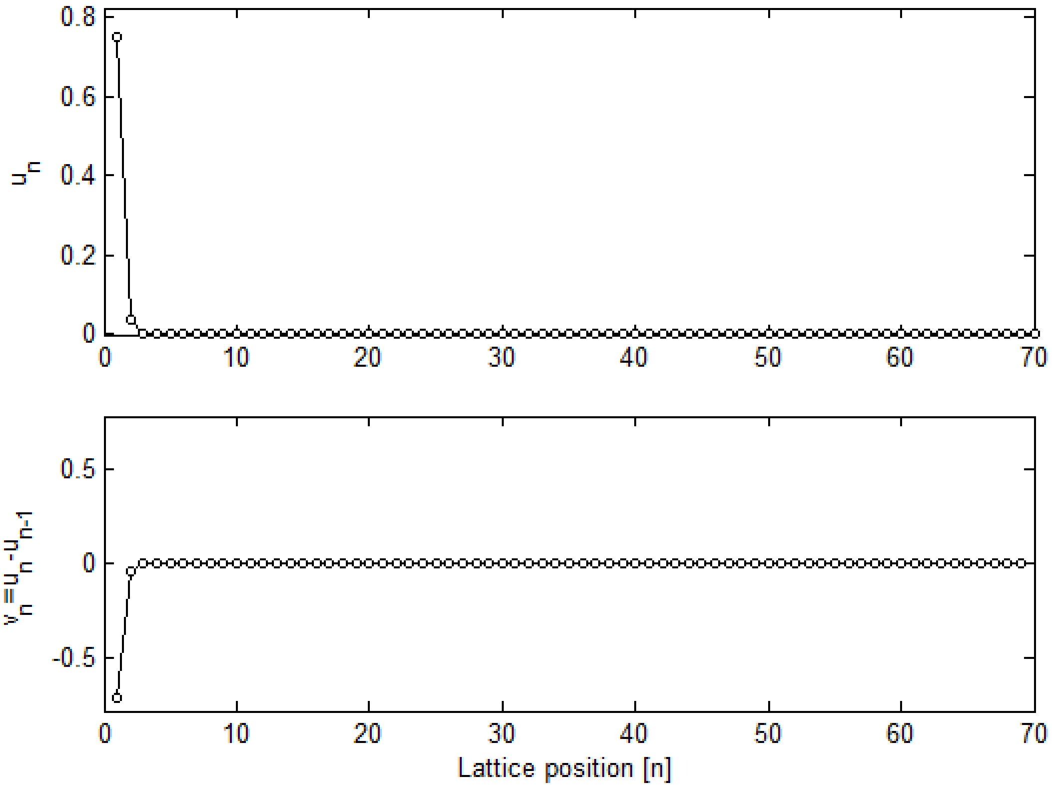




$A_0 = 1.5$

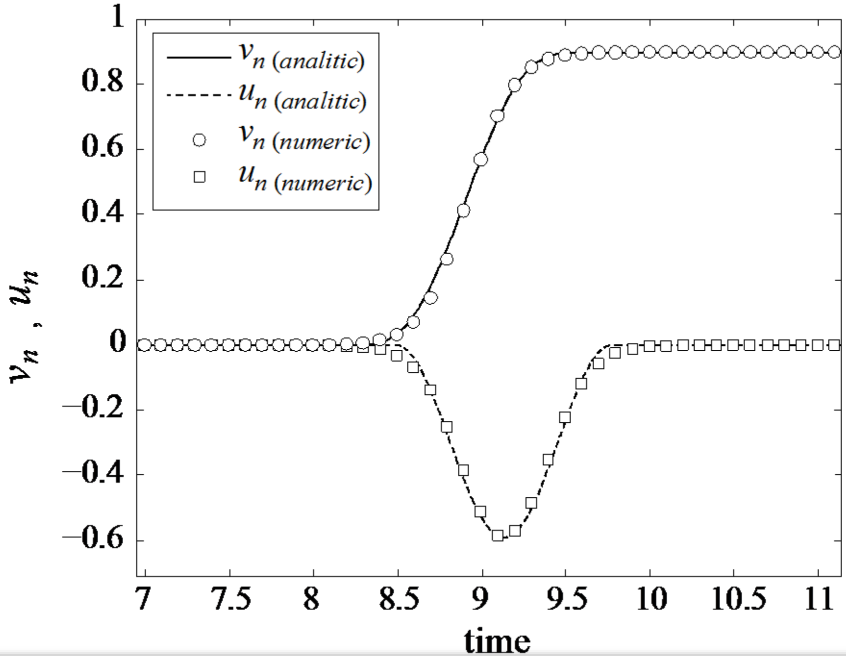
Proposed solution: for “magic” wave number $q=2\pi/3$

$$v_n(n,t) = \begin{cases} v_n = -\dfrac{A}{2}\left(1+\cos\left(qn-\omega t\right)\right) & \text{if} \quad -\pi<\left(qn-\omega t\right)<\pi \\ v_n = 0 & \text{rest} \end{cases}$$

- Rotating Wave Approximation

$$\boxed{V = \frac{1}{\left(1-A^{3/4}\right)}\, c\, \frac{\sin\left(q/2\right)}{q/2}}$$

Kinks are supersonic

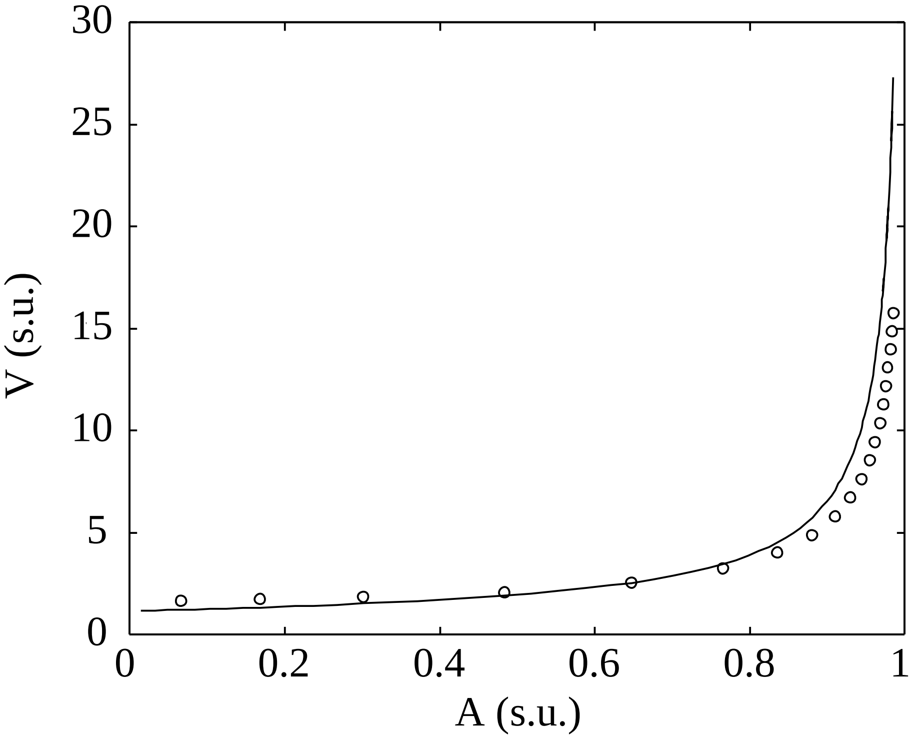


Kinks with the rotating wave approximation: *Speed vs. Amplitude*

$$V = \frac{1}{\left(1-A^{3/4}\right)} c \frac{\sin\left(q/2\right)}{q/2}$$

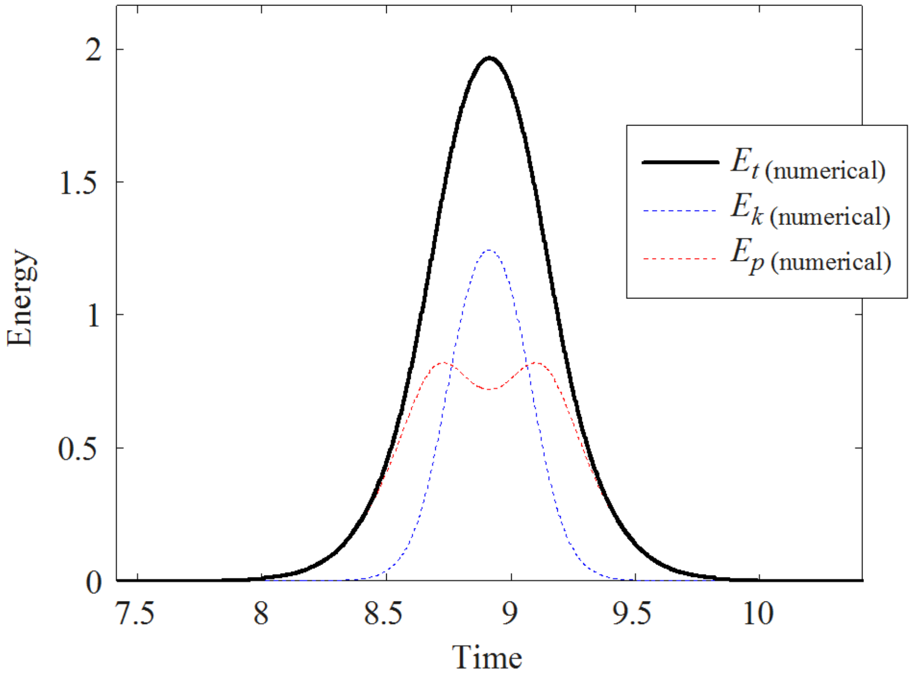
- Magic wave number $q=2\pi/3$

$$\mathrm{V} = \frac{3\sqrt{3c}}{2\pi\left(1-A\right)^{3/4}}$$



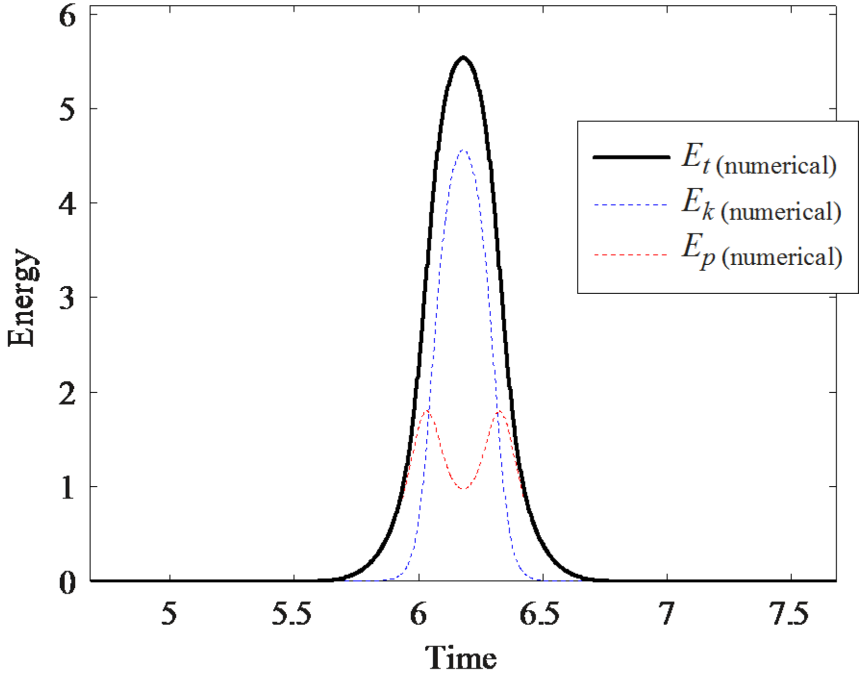
Energy vs. time

- A=0,45



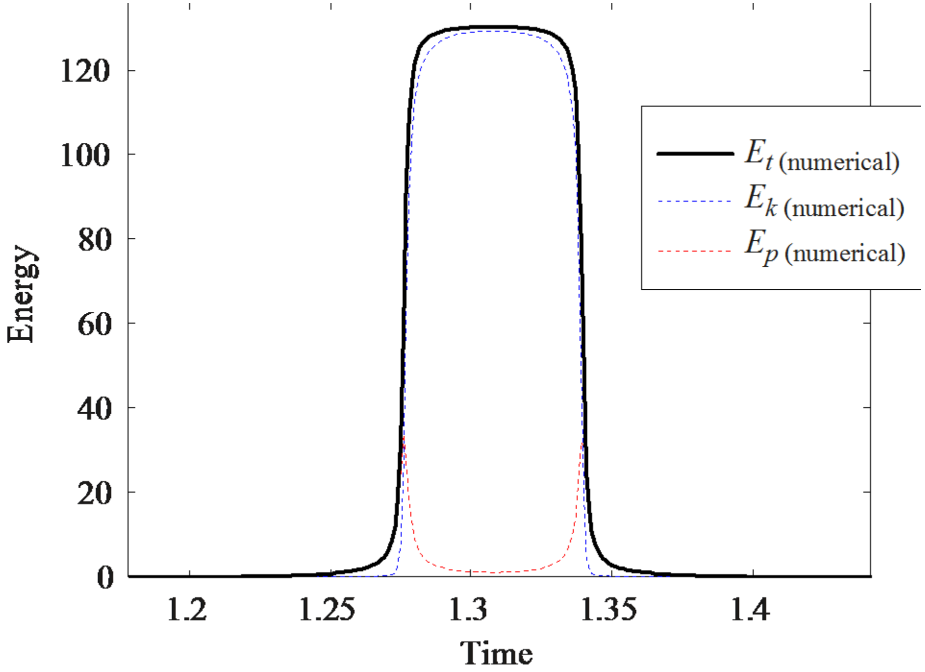
Energy vs. time

- A=0,78



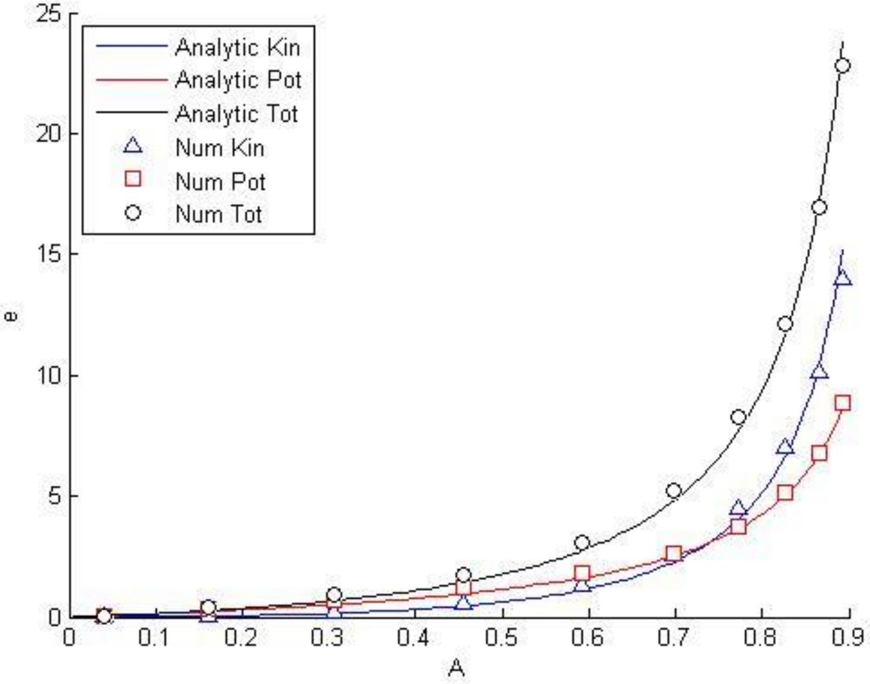
Energy vs. time

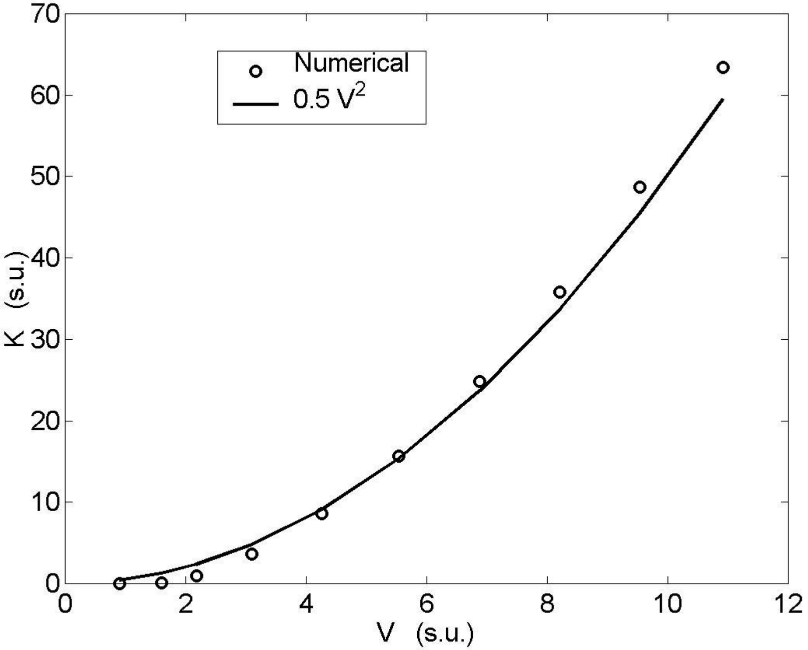
- A=0,95



A packet of energy is travelling though the chain

Energy

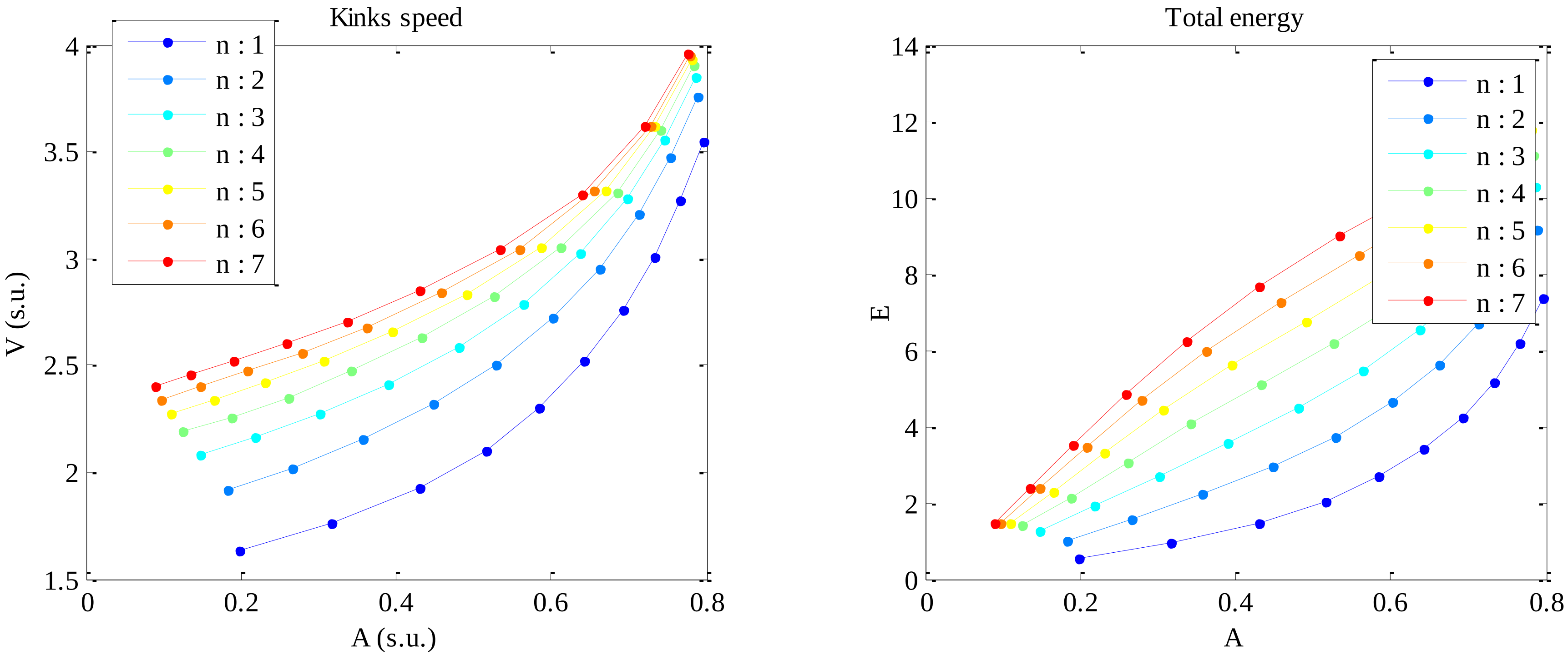




Kinks behave as particles
with unit mass

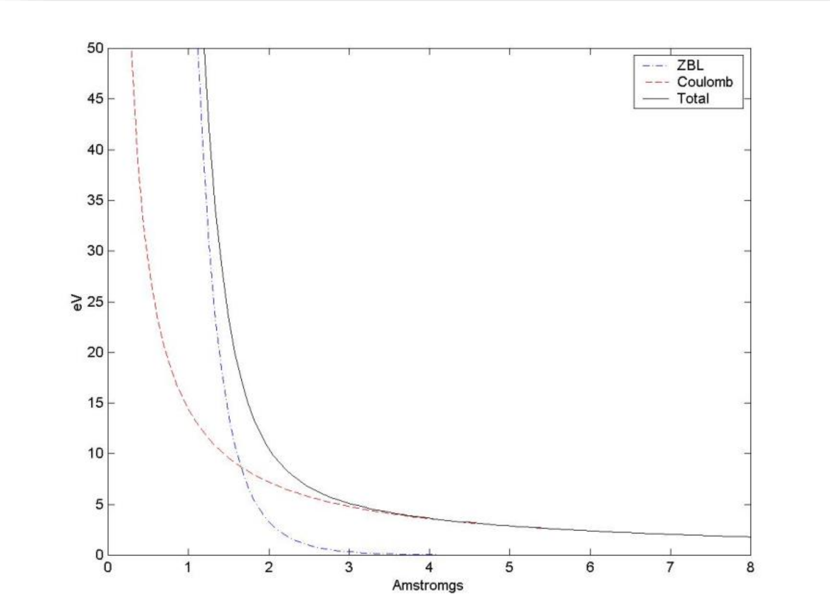
Long range interactions (N - neighbors)

- Up to 30 neighbors, kinks have been obtained



The distances between atoms are not realistic

- Short range potential: **Ziegler Biersack Litmark (ZBL):** high energy collisions
- Up to 200 keV

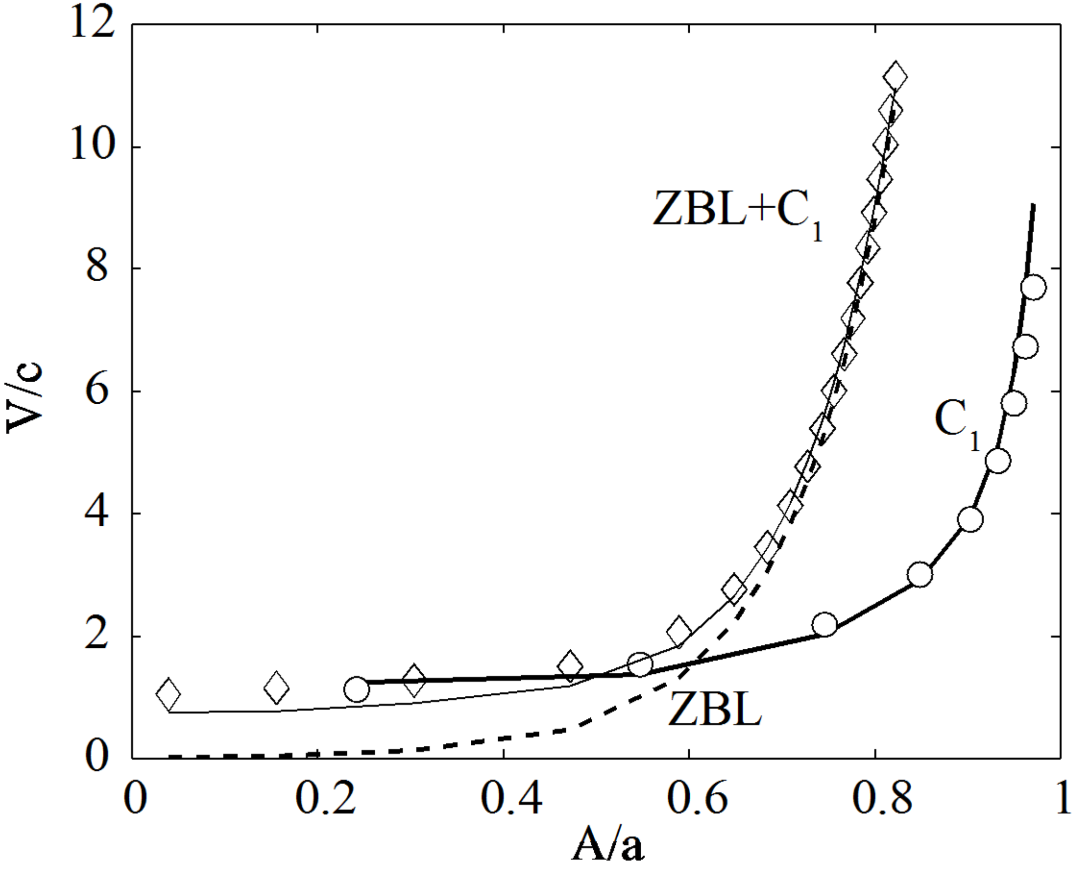


$$V(r) = \frac{2650\mathrm{eVA}}{r}\exp(-\frac{\mathrm{r}}{0.3\mathrm{A}})$$

$$V(x) = \frac{184}{x}\exp(-\frac{\mathrm{x}}{0.06})$$

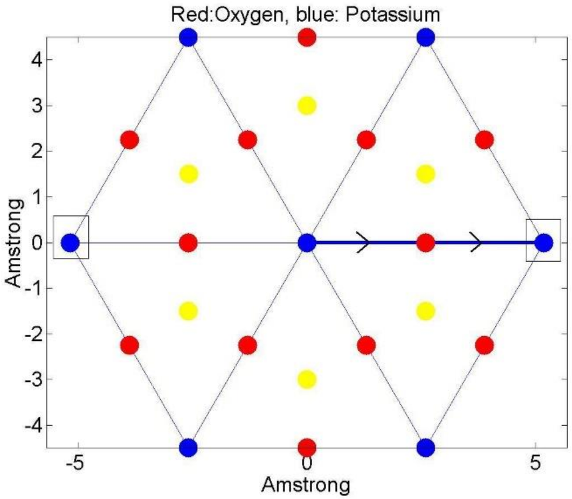
Ziegler JF, Biersack JP, Littmark U, The Stopping and Range of Ions in Matter (Pergamon, New York, 1985)

Speed (ZBL + Coulomb)



Substrate potential

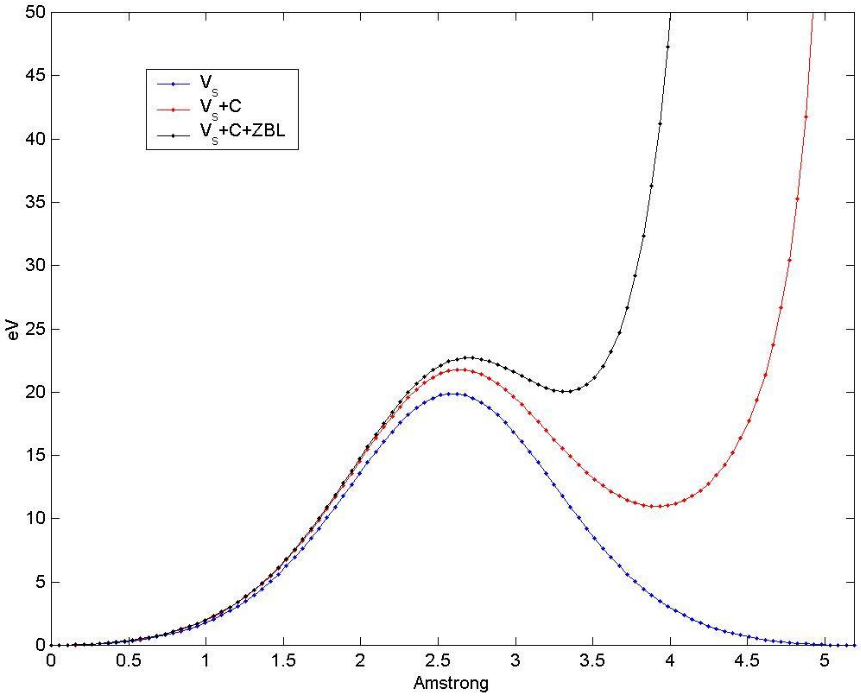
- Coulomb and Born Mayer potentials (Russell&Collins, Rad. Meas. 25, 667 (1995))



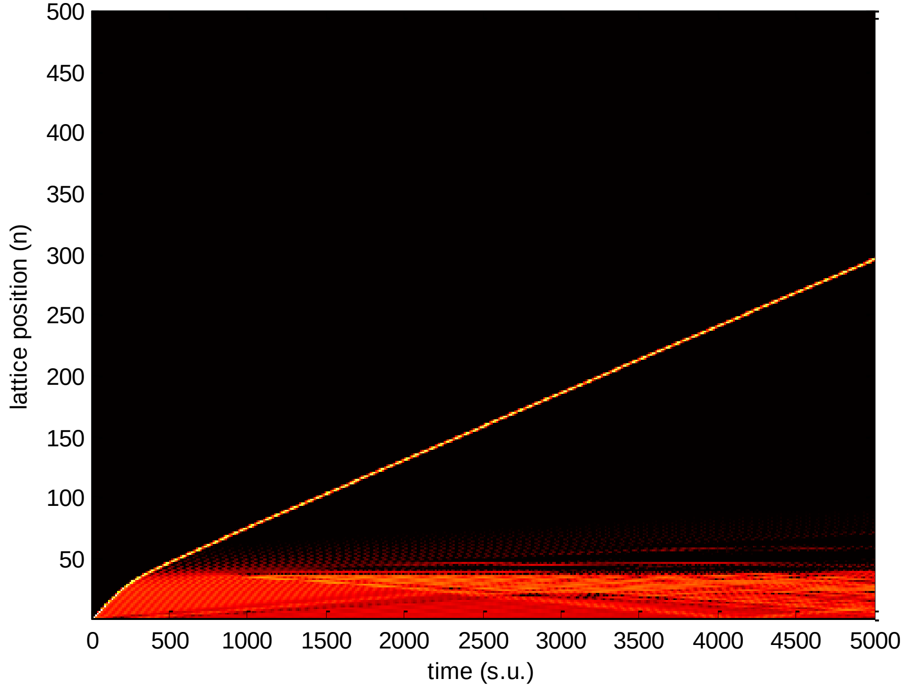
K^{+} ●

O^{-2} ●

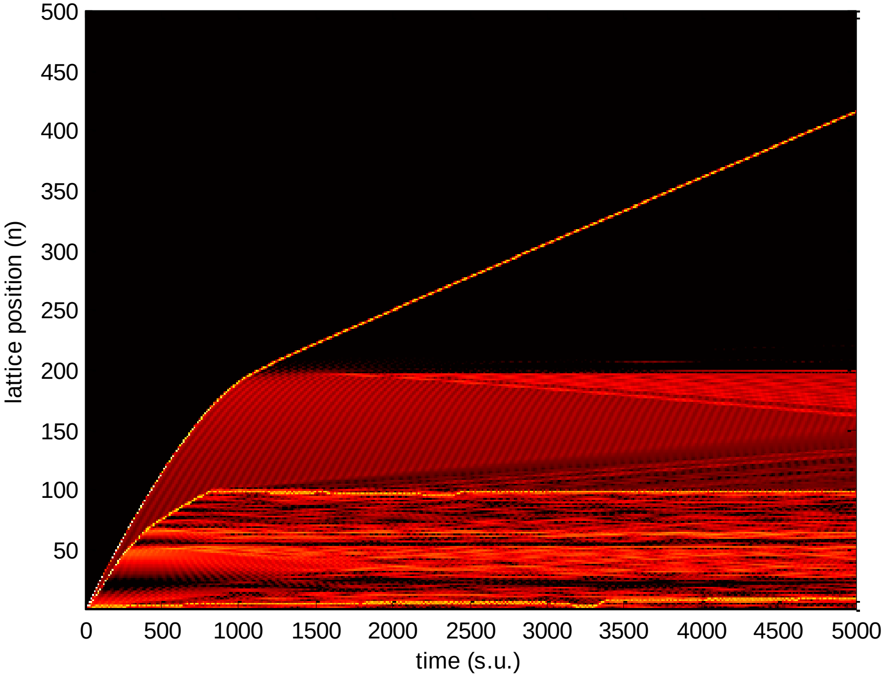
$Si^{+2.75}$ ●



Substrate potential : Energies

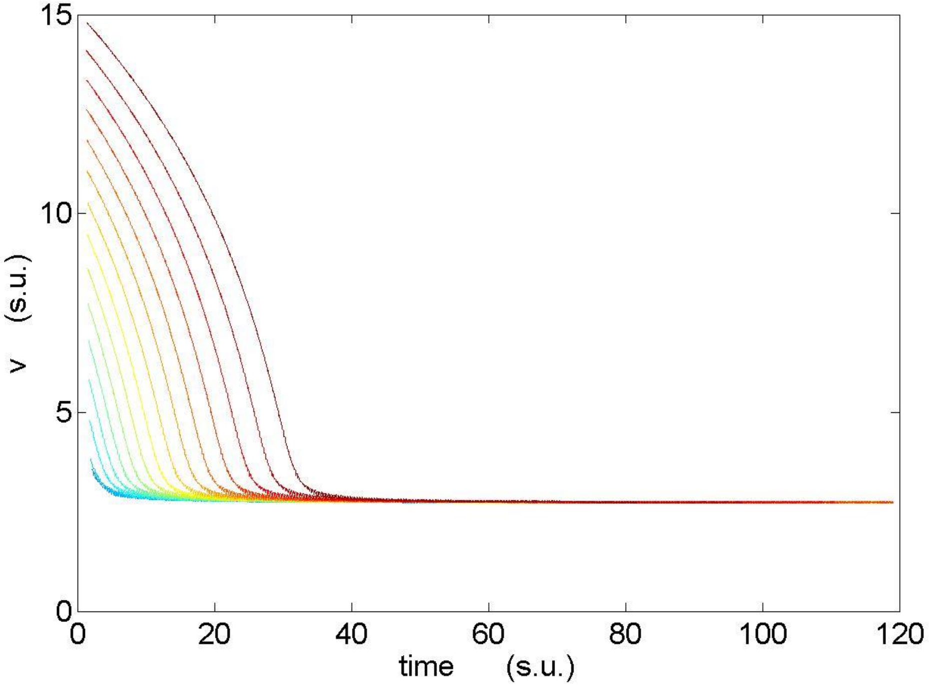


$A_{init} = 0.7 \qquad A_{end} = 0.6705$



$A_{init} = 0.8 \qquad A_{end} = 0.6705$

Lattice kinks or **Crowdions** with limit velocity



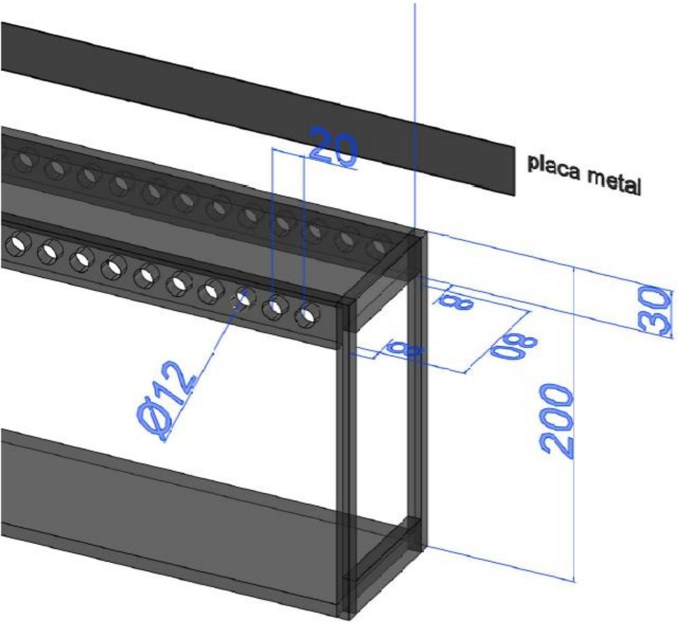
V ~2c = 8km/s , E=28 eV

- Recoil of K+ is 40 eV.
- Typical ejection energies are between 3-8 eV.

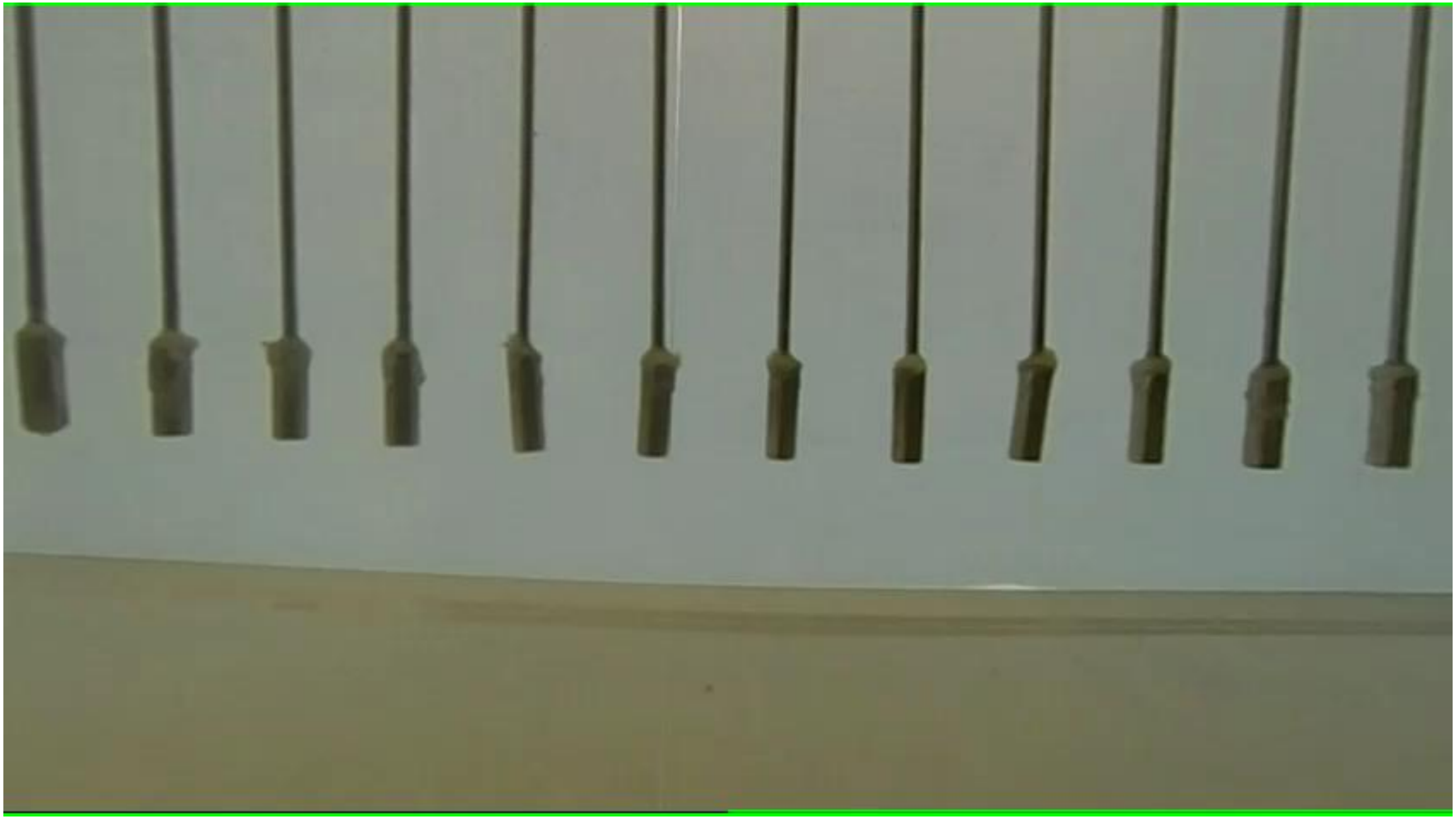
Crowdions in MD for Ni in 2D and 3D:
AM Iskandarov, Comp. Mat. Sci (2009) 429

Experimental setup:

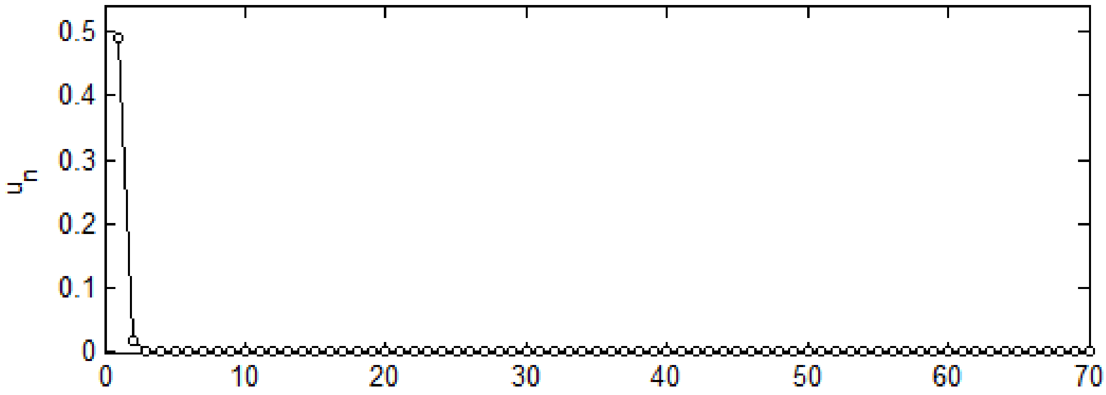
- Linear chain of 74 magnets
- Passive magnetic bearing

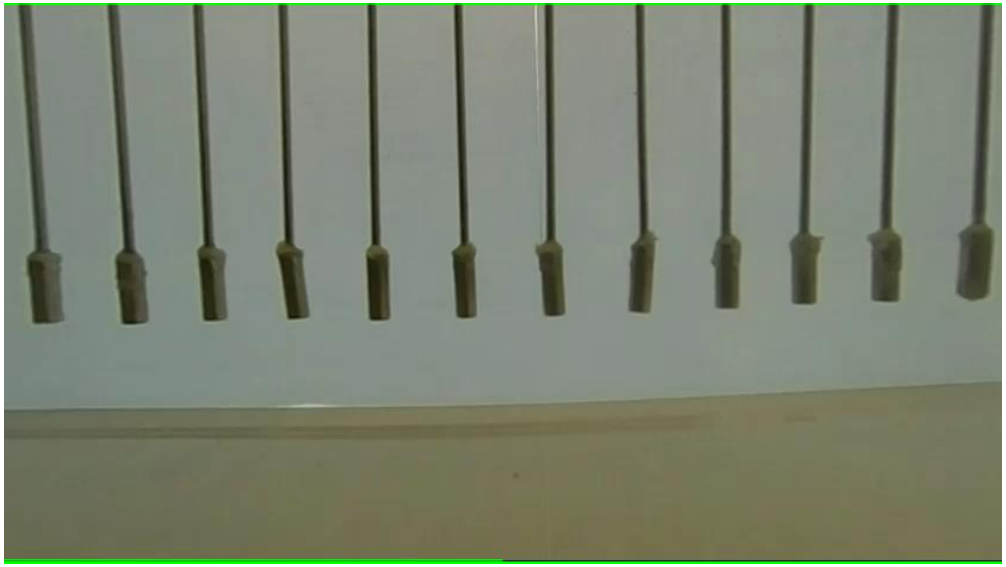


Experimental setup



Experimental setup





Experimental setup

Conclusions

- Mica has a recording capability of charged particles and lattice excitations
- There is something energetic and localized propagating in the layers of muscovite
- The are very energetic and localized lattice kinks travelling in Coulomb's chains with muscovite parameters, with properties well described by the theory, numeric and observed in toy-model experiments
- Lattice kinks select their unique own energy and velocity.
- The energy of the lattice kinks is between the surface binding energy and the energy available from K^{40} decay.
- **Coulomb's lattice kinks are candidates for *quodons***

References

- Kosevich, Yu. A., Khomeriki, R. & Ruffo, S. (2004). Supersonic discrete kink-solitons and sinusoidal patterns with “magic” wave number in anharmonic lattices, Europhys, Lett. 66, 21-27.

- Dubinko, V.I., Selyshchev, P. A. & Archilla, J.F.R. (2011). Reaction rate theory with account of the crystal anharmonicity. Phys Rev E 83, 041124,1-13.

- Russell, F. M. & Eilbeck, J. C. (2007). Evidence for moving breathers in a layered crystal insulator at 300K. Europhys, Lett., 78, 10004,1-5.

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Thanks for your attention

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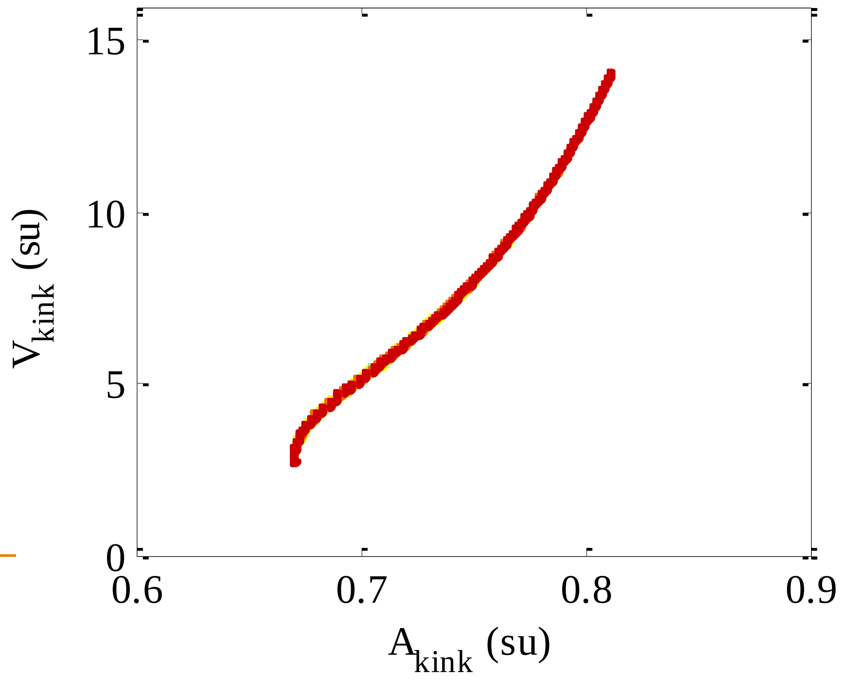
Potencial sustrato: Energías



fonón ←

Kinks estables

Radiación fonones

$$A_{end} = 0.6705$$

¿Es tan “mágico” $q=2\pi/3$?

$$V=\frac{1}{\left(1-A^{3/4}\right)}c\frac{\sin\left(q/2\right)}{q/2}$$

- Numero de onda numérico