Nuclear Fusion of Hydrogen Isotopes Induced by the Phason Flips in Pd and Ni Nanoclusters:

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Outline

- Quantum tunneling induced by time-periodic driving of the potential landscape
- Discrete Breathers in Ni and Pd hydrides
- Phason Flips in Pd and Ni nanoclusters
- Phase diagram of Pd and Ni nanoclusters loaded with hydrogen
- Low Energy Nuclear Reactions (?)
Why LENR is unbelievable?


\[ G \approx \exp \left\{ -\frac{2}{\hbar} \int_{r_0}^{R_c} dr \sqrt{2\mu(V(r)-E)} \right\} \]  
Gamow factor

\[ r_0 \sim 3 \text{ fm} \]  
Nuclear radius deduced from scattering experiments

\[ V(R_0) = \frac{e^2}{r_0} \approx 450 \text{ keV} \]  
Coulomb barrier

At any crystal Temperature:

\[ E \ll V(r_0) \Rightarrow G \approx 10^{-2760} \]

However, is the Coulomb barrier that huge in the lattice?
Willis Eugene *Lamb*
Nobel Prize 1955

Julian Schwinger
Nobel Prize 1965

*Electron screening*

J. Schwinger, Nuclear Energy in an Atomic Lattice (1990)
*Screening due to lattice oscillations*
Effective Coulomb repulsion with account of Zero-Point Oscillations

\[ 0 \langle V_c (r) \rangle_0 = \frac{e^2}{r} \sqrt{\frac{2}{\pi}} \int_0^{r/\Lambda_0} dx \exp\left(-\frac{1}{2} x^2\right) \approx \begin{cases} r \gg \Lambda_0 : \frac{e^2}{r} \\ r \ll \Lambda_0 : \left(\frac{2}{\pi}\right)^{1/2} \frac{e^2}{\Lambda_0} \end{cases} \sim 100 \text{ eV} \]

D-D fusion rate in Pd-D lattice: \( \nu_{D-D} = \frac{1}{T_0} = (2\pi/\hbar)_0 \langle V \delta(H - E)V \rangle_0 \)

\( T_0 \) is the mean lifetime of the phonon vacuum state before releasing the nuclear energy **directly** to the lattice (**no radiation!**):

\[
\frac{1}{T_0} \approx 2\pi \omega_0 \left( \frac{2\pi\hbar \omega_0}{E_{\text{nucl}}} \right)^2 \left( \frac{r_{\text{nucl}}}{\Lambda_0} \right)^3 \exp \left[ -\frac{1}{2} \left( \frac{R_0}{\Lambda_0} \right)^2 \right] \sim 10^{-19} \text{s}^{-1} \div 10^{-30} \text{s}^{-1}
\]

\( \Lambda_0 = 0.1A \)  
\( R_0 = 0.94A \div 2.9A \)
When we heat the system we increase temperature, i.e. we increase the *thermal* noise strength

Can we increase the *quantum* noise strength, i.e. ZPO energy and amplitude?
Stationary harmonic potential

\[ \langle E \rangle_n = \hbar \omega_0 \left( n + \frac{1}{2} \right) \]

\[ E_{ZPO} = \frac{\hbar \omega_0}{2} \]
Time-periodic modulation of the **double-well** shape changes (i) eigenfrequency and (ii) position of the wells
Parametric resonance with 
time-periodic eigenfrequency $\Omega = 2\omega_0$

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + \frac{m\omega^2(t)}{2} x^2 \psi$$

Schrödinger equation

$$\psi(x_0, t_0 = 0) = \frac{1}{\sqrt[4]{2\pi\sigma_0}} \exp\left(-\frac{x_0^2}{4\sigma_0}\right)$$

Initial Gaussian packet $\sigma_0 = \frac{\hbar}{2m\omega_0}$

Parametric regime $\Omega = 2\omega_0$:

$$\ddot{x} + \omega_0^2 \left[1 - g \cos(2\omega_0 t)\right] x = 0$$

g $\ll$ 1 – modulation amplitude

$$\sigma_x(t) = \sigma_0 \cosh\left(\frac{g\omega_0 t}{2}\right) \left[1 + \tanh\left(\frac{g\omega_0 t}{2}\right) \sin(2\omega_0 t)\right]$$

dispersion

ZPO energy:

$$\langle E \rangle = \frac{1}{2m} \sigma_p^2 + \frac{m\omega^2(t)}{2} \sigma_x^2 = \frac{\hbar\omega_0}{2} \cosh \frac{g\omega_0 t}{2}$$

ZPO amplitude:

$$\Lambda_{ZPO}(t) = \sqrt{\frac{\hbar}{2m\omega_0} \cosh \frac{g\omega_0 t}{2}}$$
Non-stationary harmonic potential with time-periodic eigenfrequency $\Omega = 2\omega_0$

$$\Lambda_{ZPO}(t) = \sqrt{\frac{\hbar}{2m\omega_0}} \cosh \frac{g\omega_0 t}{2}$$

$$E_{ZPO}(t) = \frac{\hbar \omega_0}{2} \cosh \frac{g\omega_0 t}{2}$$
Non-stationary harmonic potential with time-periodic shifting of the well position at $\Omega = \omega_0$

$$\langle E \rangle = \frac{\hbar \omega_0}{2} + \left( g_A A_{ZPO} \right)^2 \frac{m \omega_0^2}{8} \left[ \omega_0^2 t^2 + \omega_0 t \sin 2 \omega_0 t + \sin^2 \omega_0 t \right]$$

$$\lambda(t) = \frac{g_A A_{ZPO}}{2} \omega_0 t \left( \cos \omega_0 t - \sin \omega_0 t \right)$$
Numerical solution of non-stationary Schrödinger Equation

\[ i\hbar \frac{\partial}{\partial t} \psi(x, t) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi(x, t) + V(x, t)\psi(x, t) \]

Time-periodic double-well potential:

\[ V(x, t) = \frac{\hbar\omega_0}{2} \left[ a(t) \left( \frac{x}{\xi} \right)^4 - b(t) \left( \frac{x}{\xi} \right)^2 \right] = \frac{\hbar\omega_0}{2} u(\tilde{x}, \tau) \]

\[ a(t) = \frac{\alpha - \beta \cos(\varepsilon\omega_0 t)}{2\sqrt{\alpha}}, \quad b(t) = \frac{\sqrt{\alpha - \beta \cos(\varepsilon\omega_0 t)}}{2\sqrt{\alpha}} \]

\[ \varepsilon = 1 \div 2, \]
Initial condition: Gauss wave function

\[ \psi_R (\bar{x}, 0) = \begin{cases} \frac{1}{\sqrt{\pi \sigma^2}} \exp \left( -\frac{1}{2} \left( \bar{x} - \bar{S}_x \right)^2 \right), & -N < \bar{x} < +N \\ 0, & 0, |\bar{x}| \geq N \end{cases} \]

, \psi_I (\bar{x}, 0) = 0

\[ \tilde{S}_x = \hat{x}^{(-)} = -\frac{1}{\sqrt{2^{\frac{3}{2}} \sqrt{\alpha}}} \]

Initial wave function

Initial probability density
\( \alpha = 0.0005 \quad \beta = 0.0 \)

Stationary double-well potential

\( 0-500T \)

\( \alpha = 0.0005 \quad \beta = 0.0001 \)

Non-Stationary double-well potential

\( 0-500T \)
Probabilities to find a particle in the left (PL) or right (PR) well for the case of the Nonstationary double-well potential
Energy evolution in time-periodic double-well potential:

\[ \sigma_x = \langle (x - \langle x \rangle)^2 \rangle, \quad \sigma_x = \langle (p - \langle p \rangle)^2 \rangle, \]

\[ \langle E \rangle = \frac{1}{2m} \sigma_p + \frac{m\omega^2(t)}{2} \sigma_x \]

\[ \alpha = 0.0005 \quad \beta = 0.0001 \]

\[ V_{\text{eff}}(r) \approx \frac{m\omega_0^2}{2} r^2 + \frac{e^2}{R_0 - r} \exp\left(-\frac{R_0 - r}{\lambda_D}\right) \sqrt{\frac{2}{\pi}} \int_0^{R_0 - r/\Lambda_0} dx \exp\left(-\frac{1}{2} x^2\right) \]

Dubinko, Laptev (2016):

\[ \Lambda_0 = \frac{\hbar}{2m\omega_0} \cosh \frac{g\omega_0 t}{2} \]

Dubinko, Laptev, *Chemical and nuclear catalysis driven by LAVs*, LetMat (2016)

\[
\frac{1}{T} \approx 2\pi\omega_0 \left( \frac{2\pi\hbar \omega_0}{E_{nucl}} \right)^{\frac{1}{2}} \left( \frac{r_{nucl}}{\Lambda} \right)^3 \exp \left[ -\frac{1}{2} \left( \frac{R_0}{\Lambda_0} \right)^2 \right]
\]

\[
\Lambda_0 = \sqrt{\frac{\hbar}{2m\omega_0}} = \text{const} \\
\sqrt{\frac{\hbar}{2m\omega_0}} \cosh \frac{g \omega_0 t}{2}
\]
In order to increase probability of nuclear fusion we need a mechanism of time-periodic driving of the potential landscape

- Discrete Breathers in periodic crystals
- Phasons Flips in nanocrystals
- etc
MD modeling of DBs in NiH and PdH crystals
Visualization of the Pd(Ni)H fcc Lattice (NaCl type)
The following potential was used for Ni lattice modeling in LAMMPS package:

<table>
<thead>
<tr>
<th>Material</th>
<th>File with potential used</th>
<th>The link to the corresponding publication in the literature</th>
</tr>
</thead>
</table>
Density Of States of NiH at 0 K
H-H atoms displaced along [110] in NiH at T=0K
1 H atom displaced along <110> in NiH at T=0K

T=0.5 ps, Frequency = 20THz (inside the optical band)
H-Ni-H atoms [100] and [-100] in NiH at T=0K
H-Ni-H DB in NiH with [100] polarization

Amplitude = 1.05 Å
Frequency = 32.32 THz
Period = 0.03 ps
Lifetime = 8.3 ps = 271(T)
Excitation of DB with [111] polarization in NiH
DB with [111] polarization in NiH
DB in NiH with [111] polarization

Amplitude = 0.79 Å

Frequency = 16.39 THz

Period = 0.061 ps

Lifetime > 417 ps = 6836(T)
NiH Phonon Density of States

Frequency corresponds to the gap breather

f=16.39 THz
Do DBs exist at finite $T$?
Visualization of the PdH fcc Lattice Oscillations at T=100 K
Visualization of the PdH fcc Lattice Oscillations at $T=1000K$
Gap DBs in diatomic crystals at elevated temperatures

$K_{B,n}^* / \bar{K} \approx 5.1$

t*/$\Theta \approx 70$  $\bar{K} = 0.1eV \geq 1000K$

A$_3$B type crystals $M_H / M_L = 10$

In NaI and KI crystals Hizhnyakov et al has shown that DB amplitudes along <111> directions can be as high as 1 Å, and t*/$\Theta \sim 10^4$

Lifetime and concentration of high-energy light atoms increase exponentially with increasing T
NiH MD modeling in LAMMPS package

T=1160K

Number of High-Energy States

NiH MD modeling in LAMMPS package
NiH lattice at $T=1160K$. High energy oscillations

Data for some arbitrary H atom in the Lattice

NiH MD modeling in LAMMPS package
NiH MD modeling in LAMMPS package

T = 1600 K

Number of High-Energy Oscillations

\[ \text{Number of High-Energy Oscillations} \]

\[ T = 1600 \text{ K} \]

NiH MD modeling in LAMMPS package
Wavelet imaging of LAV in NiH MD (Francesco Piazza, Nal, 2018)

The technique is based on continuous wavelet transform of velocity time series coupled to a threshold dependent filtering procedure to isolate excitation events from background noise in a given spectral region.

By following in time the center of mass of the reference frequency interval, the data can be exploited to investigate the statistics of the burst excitation dynamics, by computing, for instance, the distribution of the burst lifetimes, excitation times, amplitudes and energies.
Wavelet imaging of LAV in NiH MD (Francesco Piazza, 2018)

![Graphs showing temperature vs. various parameters including average burst kinetic energy, mean square displacement, average lifetime, and site-occupancy probability.](image-url)
In physics, the term **clusters** denotes small, multiatom particles. As a rule of thumb, any particle of somewhere between 3 and $3 \times 10^7$ atoms is considered a cluster. Two-atom particles are sometimes considered clusters as well. A two atom particle may also be a molecule.

**Nanoclusters** are particles between 1 and 100 nanometers (nm) in size with a surrounding interfacial layer. The interfacial layer is an integral part of nanoscale matter, fundamentally affecting all of its properties. The interfacial layer typically consists of ions, inorganic and organic molecules. Organic molecules coating inorganic nanoparticles are known as stabilizers, capping and surface ligands, or passivating agents. In nanotechnology, a particle is defined as a small object that behaves as a whole unit with respect to its transport and properties.
Cuboctahedral and Icosahedral clusters

**Cuboctahedral clusters (fcc)** the only spatial configuration in which the length the polyhedral edges is equal to that of the radial distance from its center of gravity to any vertex.

**Icosahedral clusters** possess 5 fold symmetry.
## Dependence of cluster diameter on number of atoms

<table>
<thead>
<tr>
<th># of atoms</th>
<th>d(Pd cubo), Å</th>
<th>d(Pd ico), Å</th>
<th>d(Ni cubo), Å</th>
<th>d(Ni ico), Å</th>
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<tbody>
<tr>
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<td>923</td>
<td>30.5118</td>
<td></td>
<td></td>
<td>28.1917</td>
</tr>
</tbody>
</table>
CUBO-ICO Structural Transformation at near 0K

Unifying motion between 4-fold (crystal) and 5-fold (quasi-crystal) symmetries

Reversible and irreversible

cuboctahedron icosahedron

Diagram showing potential energy of the Pd13 cluster over time.

-25.19 eV at -25.2 eV
-24.74 eV at 0.45 eV
-0.035 eV/atom at -25.19 eV
Time Dependence of Potential Energy for Pd13

For different clusters we analyzed the oscillations of potential energy.
CUBO-ICO Structural Transformation at near 0K
Pd13_CUBO cluster has been considered. Initial temperature was set to 0K. After that the NVE dynamics has been modeled. Time in picoseconds, energy in eV.
CUBO-ICO Structural Transformation at 30K
Pd13_cubo_nve

Pd13 CUBO cluster has been considered. Initial temperature was set to 30K. After that the NVE dynamics has been modeled. Time in picoseconds, energy in eV.
CUBO-ICO Structural Transformation at 300K
Pd13_cubo_nve

Pd13 CUBO cluster has been considered. Initial temperature was set to 300K. After that the NVE dynamics has been modeled. Time in picoseconds, energy in eV.
Temperature-driven phase transformation

- QCs of Pd exhibit temperature driven phase transformation
- Size of cluster and hydrogenization affects transformation
- Larger size – higher transformation temperature
- High Hydrogen concentration – lower transformation temperature
Temperature of the Structural Transition for Ni147 cluster. $T=133 K$

For larger clusters there exists some critical temperature for the transition. For Ni147 Structural transition was observed at $T=133 K$. For $T<133 K$ cuboctahedral cluster preserved it`s symmetry and didn`t transform to icosahedral cluster.
MD modeling of the Pd-H and Ni-H clusters heating

The heating of clusters was performed in a canonical (NVT) ensemble with Nose thermostat. During the simulation the temperature was determined by the average kinetic energy of the atoms, which was calculated using the Verlet velocity algorithm with a time step 0.0005ps = 0.5fs.

During the heating the temperature was changed from 10 to 1000K
**x-T Phase diagram for the Pd147Hx cluster**

Initial condition: cluster has cuboctahedral (CUBO) configuration. The heating of clusters was performed in a canonical (NVT) ensemble with Nose thermostat. During the simulation the temperature was determined by the average kinetic energy of the atoms, which was calculated using the Verlet velocity algorithm with a time step $0.0005\text{ps} = 0.5\text{fs}$.

As temperature ($T$) increase cluster undergoes transformation from cuboctahedral (CUBO) phase to icosahedral (ICO) phase and then to amorphous (A) phase. The further temperature increase results in melting and evaporation/sublimation processes. Clusters with different number of H atoms ($x$) have been considered.
x-T Phase diagram for the Pd147Hx cluster

Initial condition: cluster has icosahedral (ICO) configuration. The heating of clusters was performed in a canonical (NVT) ensemble with Nose thermostat. During the simulation the temperature was determined by the average kinetic energy of the atoms, which was calculated using the Verlet velocity algorithm with a time step 0.0005 ps = 0.5 fs. As temperature (T) increases cluster undergoes transformation from icosahedral (ICO) phase to amorphous (A) phase. The further temperature increase results in melting and evaporation/sublimation processes. Clusters with different number of H atoms (x) have been considered. For large x the transformation to cuboctahedral (CUBO) phase was observed.
x-T Phase diagram for the Pd561Hx cluster

Initial condition: cluster has cuboctahedral (CUBO) configuration. The heating of clusters was performed in a canonical (NVT) ensemble with Nose thermostat. During the simulation the temperature was determined by the average kinetic energy of the atoms, which was calculated using the Verlet velocity algorithm with a time step $0.0005\text{ps} = 0.5\text{fs}$.

As temperature (T) increase cluster undergoes transformation from cuboctahedral (CUBO) phase to icosahedral (ICO) phase and then to amorphouse (A) phase. The further temperature increase results in melting and evaporation/sublimation processes. Clusters with different number of H atoms (x) have been considered.
Initial condition: cluster has icosahedral (ICO) configuration. The heating of clusters was performed in a canonical (NVT) ensemble with Nose thermostat. During the simulation the temperature was determined by the average kinetic energy of the atoms, which was calculated using the Verlet velocity algorithm with a time step $0.0005$ ps = $0.5$ fs.

As temperature ($T$) increase cluster undergoes transformation from icosahedral (ICO) phase to amorphous (A) phase. The further temperature increase results in melting and evaporation/sublimation processes. Clusters with different number of H atoms ($x$) have been considered.

For large $x$ the transformation to cuboctahedral (CUBO) phase was observed.
Embedding of QCs in Zeolite

• Strategy
  – Assumption: Zeolite act as “magnetic pillow” which holds QC
  – Phase transformation of QCs will occur in similar manner inside Zeolite just as in simulated vacuum
  – Atomic force interaction (Al-Si-O-H-Pd) can be derived from Ab Initio calculations and transferred to LAMMPs tool

• Current progress
  – Trial atomic force matrix is derived
  – Trial Zeolite – Pd 13 and Pd 147 is modelled
  – Phase transformation inside Zeolite is observed
Pd13 ICO cluster inside FAU Zeolite
Pd13 ICO cluster inside FAU Zeolite
Pd55 CUBO cluster inside FAU Zeolite
Summary

- Phason flip (or phase transformation of QC cluster) is considered as a possible trigger of D-D reaction
- Phason flip was modelled in Pd and Pd-H QC clusters by LAMMPs techniques; phase diagram is obtained for the QCs of relevant size and hydrogenization
- LAMMPs technique was validated by AB INITIO code to ensure that structure and energetic stability of QC clusters is respected
- Zeolite is now modelled as “Magnetic Pillow” holding the QC cluster
- Zeolite-QC cluster interaction matrix needs to be derived using AB INITIO, and then implemented in LAMMPs tool
- Preliminary calculations show that QCs embedded in Zeolite (with simplified force matrix) also exhibit phase transformation in similar style as observed by modelling “vacuum case”
Low temperature testing of the sample S14-100 (Carbon template with 15 wt% of 1.5-17 nm Pd nanoparticles)
By Prof. Alexander Dolbin, head of the Department of Thermal properties and structure of Solids and nanosystems
Kharkov Institute of Low Temperature Physics.

The hydrogen (red) and deuterium (blue) desorption curves from S14-100 sample at \( T = 13 \text{ K} \). Sudden bursts of gas pressure during desorption of deuterium at the beginning of desorption and after 3600 s can be seen far exceeds the experimental error. A possible reason for the deuterium desorption bursts may be AHE bursts !!!
Conclusions and outlook

New mechanism of catalysis in solids is proposed, based on time-periodic driving of the potential landscape induced by Discrete Breathers.

At high T, DBs formed in Pd or Ni hydrides may result in effective lowering of the reaction activation barrier.

At low T, DBs formed in Pd or Ni hydrides and Phason Flips of 13 atom Pd or Ni clusters may result in increasing energy of Zero Point Oscillations enhancing the tunneling through the potential barrier

Outstanding problems:

Efficient methods of DB generation in Pd or Ni hydrides are needed such as electromagnetic irradiation or electric pulses

Experimental methods to synthesize 13 atom Pd or Ni clusters (sizes ~ 0.5 nm!) confined in nano-porous matrixes need to be developed
Publications

THANK YOU FOR YOUR ATTENTION!