



Research Article

Nuclear Catalysis Mediated by Localized Anharmonic Vibrations

Vladimir Dubinko*

National Science Center “Kharkov Institute of Physics and Technology”, Kharkov 61108, Ukraine

Abstract

In many-body nonlinear systems with sufficient anharmonicity, a special kind of lattice vibration, namely, Localized Anharmonic Vibrations (LAVs) can be excited either thermally or by external triggering, in which the amplitude of atomic oscillations greatly exceeds that of harmonic oscillations (phonons) that determine the system temperature. The coherency and persistence of LAVs may have a drastic effect on quantum tunneling due to correlation effects discovered by Schrödinger and Robertson in 1930. These effects have been applied to the tunneling problem by a number of authors, who demonstrated a giant increase of sub-barrier transparency during the increase of the correlation coefficient at a special high-frequency periodic action on the quantum system. Recently, it has been proposed that discrete breathers (a sub-class of LAVs arising in periodic systems) present the most natural and efficient way to produce correlation effects in regular crystals due to time-periodic modulation of the potential well (or the Coulomb barrier) width and hence to act as breather ‘nano-colliders’ catalyzing low energy nuclear reactions (LENR) in solids. It has been shown that the tunneling probability for D–D fusion under electrolysis of heavy water increases enormously with increasing number of oscillations resulting in the fusion rates comparable with those observed experimentally. In the present paper, we discuss possible ways of engineering the nuclear-active environment (NAE) and catalyzing LENR in NAE based on the LAV concept. We propose some practical ways of catalyzing LENR that are based on a special electro-magnetic treatment or electron and gamma irradiation, which could trigger LAVs in crystals and clusters.

© 2017 ISCMNS. All rights reserved. ISSN 2227-3123

Keywords: Correlation effects, Discrete breathers, Localized anharmonic vibrations, Low energy nuclear reactions, Nuclear active sites

1. Introduction

Catalysis is at the heart of almost every chemical or nuclear transformation process, and a detailed understanding of the active species and their related reaction mechanism is of great interest [1–3]. There is no single theory of catalysis, but only a series of principles to interpret the underlying processes. An important parameter of the reaction kinetics is the *activation energy*, i.e. the energy required to overcome the reaction barrier. The lower is the activation energy, the faster the reaction rate, and so a catalyst may be thought to somehow reduce the activation energy. Dubinko et al. have shown [4,5] that in a crystalline matrix, the activation energy may be reduced at some sites due to a special class of

*E-mail: vdubinko@hotmail.com.

localized anharmonic vibrations (LAV) of atoms, known also as *discrete breathers* [6] or *intrinsic localized modes* [7] arising in regular crystals. Discrete breathers (DB) can be excited thermally or by external driving, resulting in a drastic acceleration of *chemical reaction rates* in their vicinity. What is more, recently, discrete breathers have been proposed as *catalysts of nuclear D–D fusion* in palladium deuteride under heavy water electrolysis [8]. This new concept does not require any modification of *conventional nuclear physics laws*, in a marked contrast to the most of LENR models that attempted introducing various types of transient quasi-particles and structures such as Hydrino, Hydron, Hydrex, etc. that were created *ad hoc* to lower the Coulomb barrier, but which have not been verified by nuclear physics.

One of the most important practical ways to confirm the new concept is to look for the environment where the reaction is expected, which can be enriched with sites of *zero or small threshold energies* for the excitation of DBs. Such sites are expected to become the *nuclear active sites*, according to the model [8]. In this context, a striking *site selectiveness* of LAV formation in disordered structures [5] allows one to suggest that their concentration in quasicrystals may be very high as compared to regular crystals where DBs (a sub-class of LAV) arise homogeneously, and their activation energy is relatively high. Direct experimental observations [9] have shown that in the decagonal quasicrystal $\text{Al}_{72}\text{Ni}_{20}\text{Co}_8$, *mean-square thermal vibration amplitude* of the atoms at special sites greatly exceeds the mean value, and the difference increases with temperature. This might be the first experimental observation of LAV, which has shown that they are arranged just a few nanometers from each other, which means that their average concentration was about 10^{20} per cubic cm, which is orders of magnitude higher than one could expect to find in periodic crystals [4,5,8]. So in this case, one deals with a kind of ‘*organized disorder*’ that stimulates formation of LAV, which may explain the strong catalytic activity of some quasicrystals and open new ways towards *engineering of NAE* based on computer modeling of LAVs in periodic and aperiodic crystals and nano clusters. The main goal of the present paper is to develop this concept to the level of quantitative comparison with some of the LENR experiments and to suggest some practical ways of catalyzing LENR.

This paper is organized as follows. In Section 2, we briefly discuss the problem of tunneling through the Coulomb potential barrier, taking into account the *correlation effects*, as proposed by Dodonov et al. [10] and more recently by Vysotskii et al. [11]. A giant increase of sub-barrier transparency (up to hundreds of orders of magnitude) during the increase of the correlation coefficient at special periodic action on a quantum system will be demonstrated.

In Section 3, we will show that such an action can be most naturally achieved with time-periodic modulation of the width of potential wells for atoms oscillating in the vicinity of a *DB* or, more generally, LAV. We find the critical parameters of LAVs required to form *coherent correlated states* (CCS) via ‘parametric resonance’ conditions.

In Section 4, based on the LAV concept, an alternative to heating (currently used for triggering LENR) is proposed that is based on a special electro-magnetic treatment or electron irradiation, which can trigger LAVS in crystals and clusters and thus catalyze LENR. Methods of experimental verification of the proposed concept are discussed in Section 5. A summary and outlook is given in Section 6.

2. Tunneling enhancement due to formation of CCS in non-stationary potential well

2.1. Heisenberg uncertainty relation, Gamow TC and screening potential effects

The problem of tunneling through the Coulomb potential barrier during the interaction of charged particles is the key to modern nuclear physics, especially in connection with low energy nuclear reactions (LENR) observed in solids [12–14].

The tunneling (a.k.a. transmission) coefficient (TC) first derived by Gamow (1928) for a pure Coulomb barrier is

the Gamow factor, given by

$$G \approx \exp \left\{ -\frac{2}{\hbar} \int_{r_1}^{r_2} dr \sqrt{2\mu (V(r) - E)} \right\}, \quad (1)$$

where $2\pi\hbar$ is the Planck constant, E is the nucleus CM energy, μ is the reduced mass, r_1, r_2 are the two classical turning points for the potential barrier, which for the D–D reaction are given simply by $\mu = m_{\text{D}}/2$, $V(r) = e^2/r$. For two D's at room temperature with thermal energies of $E \sim 0.025$ eV, one has $G \sim 10^{-2760}$, which explains the pessimism about whether LENR can exist, and shows the need for some *special conditions* arising in solids under typical LENR conditions (D₂O electrolysis [12,13] or Ni–H reaction [14], etc.), which help to overcome the Coulomb potential.

Corrections to the cross section of fusion due to the screening effect of atomic electrons result in the so-called “*screening potential*”, which acts as an additional source of energy of collisions at the center of mass [15]. The screening potential was measured by the yields of protons or neutrons emitted in the D(d, p)T or D(d, n)³He reactions induced by bombardment of D-implanted solid targets with deuterons accelerated to kinetic energies of several keV, equivalent to heating up to $\sim 10^7$ K [16]. However, even the maximum screening potentials found in Pt (675 eV), PdO (600 eV) and Pd (310 eV) are far too weak to explain LENR observed at the temperatures of the experiments, which are below melting point of solids. Besides, the absence of significant radiation under typical LENR conditions indicates that *other reactions* should take place, based on interactions between ‘slow’ particles, which may be qualitatively different from the interactions between accelerated ones.

The most promising and universal mechanism of the stimulation of nuclear reactions occurring at low energy is connected with the formation of *coherent correlated states* of interacting particles, which ensures the large probability of nuclear reactions under these conditions, where the ordinary tunneling probability is negligible. These states minimize a more general uncertainty relation (UR), rather than the Heisenberg UR usually considered in quantum mechanics, namely, Schrödinger–Robertson UR [17,18], which takes into account *correlations between coordinate and momentum operators*.

2.2. Schrödinger–Robertson uncertainty relation and TC

The tunneling effect for nuclear particles is closely related to the uncertainty relation (UR), which determines, in fact, the limits of the applicability of the classical and quantum descriptions of the same object. It appears that the well-known and widely used Heisenberg UR is a special case of a more general inequality, discovered independently by Schrödinger [17] and Robertson [18], which can be rewritten in the following form [10,19]

$$\sigma_x \sigma_p \geq \frac{\hbar^2}{4(1-r^2)}, \quad r = \frac{\sigma_{xp}}{\sqrt{\sigma_x \sigma_p}}, \quad \sigma_{xp} = \langle \hat{x}\hat{p} + \hat{p}\hat{x} \rangle / 2 - \langle \hat{x} \rangle \langle \hat{p} \rangle, \quad (2)$$

$$\sigma_x = \left\langle (x - \langle x \rangle)^2 \right\rangle, \quad \sigma_p = \left\langle (p - \langle p \rangle)^2 \right\rangle, \quad (3)$$

where r is the *correlation coefficient* between the coordinate, x , and momentum, p , operators. At $r = 0$ (non-correlated state) Eq. (2) is reduced to the Heisenberg UR, while in a general case, a nonzero r in the UR can be taken into account by the formal substitution

$$\hbar \rightarrow \hbar_{\text{ef}} = \frac{\hbar}{\sqrt{1-r^2}}, \quad (4)$$

which leads to the formal shift of the border between the classical and quantum descriptions of the same object in the transition from noncorrelated to correlated state [11].

Then a natural question arises: can non-zero correlations lead to real physical effects? *The answer is yes*, and the most impressive consequence is a dramatic increase of the tunneling probability, if a real Planck constant in Eq. (1) can be replaced by the effective parameter (4). This substitution was indeed justified for a very low tunneling probability in the initially uncorrelated state $G_{r=0} \ll 1$ that corresponds to the condition $E \ll V_{\max}$ [11]:

$$G_{r \neq 0} \approx \exp \left\{ -\frac{2}{\hbar_{\text{ef}}} \int_{r_1}^{r_2} dr \sqrt{2\mu(V(r) - E)} \right\} = (G_{r=0})^{\sqrt{1-r^2}}. \quad (5)$$

From Eq. (5), it follows that when a strongly correlated state with $|r| \rightarrow 1$ is formed, the product of the variances of the particle coordinate and momentum increases indefinitely, and the barrier becomes practically ‘transparent’: $G_{|r| \rightarrow 1} \rightarrow 1$ even if $E \ll V_{\max}$.

Although the substitution $\hbar \rightarrow \hbar_{\text{ef}}$ (4) is not quite correct quantitatively, it clearly demonstrates the high efficiency of the correlations in applied tunneling-related problems in the case of a high potential barrier and a low particle energy $E \ll V_{\max}$, which is typical for LENR.

The physical reason for the huge increase in barrier transparency for a particle in a CCS is the *co-phasing* of all fluctuations of the momentum for various eigenstates forming the superpositional correlated state, which leads to great dispersion of momentum and large fluctuations of positions of a particle in the potential well and *under the potential barrier*.

A CCS can be formed in various quantum systems. The most effective way to form such state is to place a particle in a *non-stationary potential well*. Exact solutions to the non-stationary Schrödinger equation for the oscillating particle wave function $\psi(x, t)$ have been found by Vysotskii et al. [11], which will be considered in the following section.

2.3. Formation of CCS under time-periodic action on a particle in the parabolic potential

Consider a harmonic oscillator in a non-stationary potential well with eigenfrequency $\omega(t)$ changing with time, t , the Hamiltonian of which is given by

$$\hat{H} = \frac{\hbar}{2M} \frac{\partial^2}{\partial x^2} + \frac{M\omega(t)^2 x^2}{2}. \quad (6)$$

The solution of the Schrödinger equation for this Hamiltonian by Dodonov and Man’ko [10,19] gives the wave function of the correlated state having the time-periodic oscillating dispersion of the particle coordinate $\sigma_x(t)$:

$$\Psi_{\text{corr}}(x, t, r) = \frac{1}{\sqrt[4]{2\pi\sigma_x(t)}} \exp \left[-\frac{x^2}{4\sigma_x(t)} \left(1 - \frac{ir(t)}{\sqrt{1-r^2(t)}} \right) \right], \quad \sigma_x(t) = \frac{x_0^2}{2\sqrt{1-r^2(t)}}, \quad (7)$$

where $x_0 = \sqrt{\hbar/M\omega_0}$ is the amplitude of zero-point oscillations, which shows the scaling of the quantum problem. With increasing $|r| \rightarrow 1$ the dispersion increases indefinitely, which means that a probability of the particle localization in the sub-barrier region increases accordingly. For example, $x_0 \approx 0.56 \text{ \AA}$ for a hydrogen nucleus, and the probability of its tunneling to a distance comparable with the crystal lattice spacing (on the order of angstroms) drastically increases with increasing $|r|$.

A model system considered by Vysotskii et al. [11] to evaluate the correlation coefficient is a particle with the mass M , coordinate $x(t)$ and momentum $p(t)$ in a non-stationary parabolic potential well (i.e. non-stationary harmonic

oscillator),

$$V(x, t) = M(x(t))^2(\omega(t))^2/2, \quad (8)$$

for which a change of the eigenfrequency $\omega(t)$ was shown to result in an increase of the absolute value of $|\psi(t)|$. Several scenarios of time evolution $\omega(t)$ have been investigated [11], including its monotonic decrease or periodic modulation. The latter regime can be provided, e.g. at a constant well depth V_{\max} if the potential well width $L(t)$ changes periodically resulting in a time-periodic modulation of the eigenfrequency as follows:

$$L(t) = L_0(1 + g_\Omega \cos \Omega t), \quad L_0 = \sqrt{8V_{\max}/M\omega_0^2}, \quad (9)$$

where L_0 and ω_0 are the initial parameters of the well before the action of correlated forces, g_Ω and Ω are the modulation amplitude and frequency, respectively.

From a detailed analysis [11] it follows that the process of formation of strongly correlated coherent state with $|\psi|_{\max} \rightarrow 1$ in response to the action of limited periodic modulation is possible only at any of two conditions: (i) $\Omega = \omega_0$ (resonant regime) or (ii) $\Omega \approx 2\omega_0$, $|\Omega - 2\omega_0| \leq g_\Omega\omega_0$ (parametric regime). An analytical solution of the Schrödinger equation in the parametric regime was obtained by Dubinko, Laptev [20]. It shows that parametric modulation of a parabolic potential well results in the increase of the coordinate, momentum and mutual dispersion with increasing number of oscillation periods, N , which results in rapidly increasing probability to find the oscillating particle far beyond the characteristic length of the stationary well $\xi = \sqrt{\hbar/M\omega_0}$ (Fig. 1).

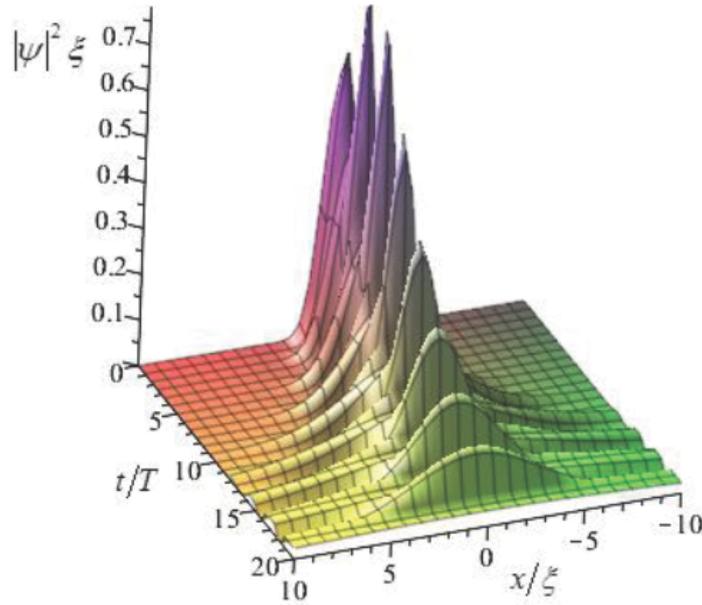


Figure 1. Localization probability distribution vs. the number of oscillation periods $N = \omega_0 t/2\pi = t/T$ in the parametric regime $\Omega = 2\omega_0$ at $g_\Omega = 0.1$ [20].

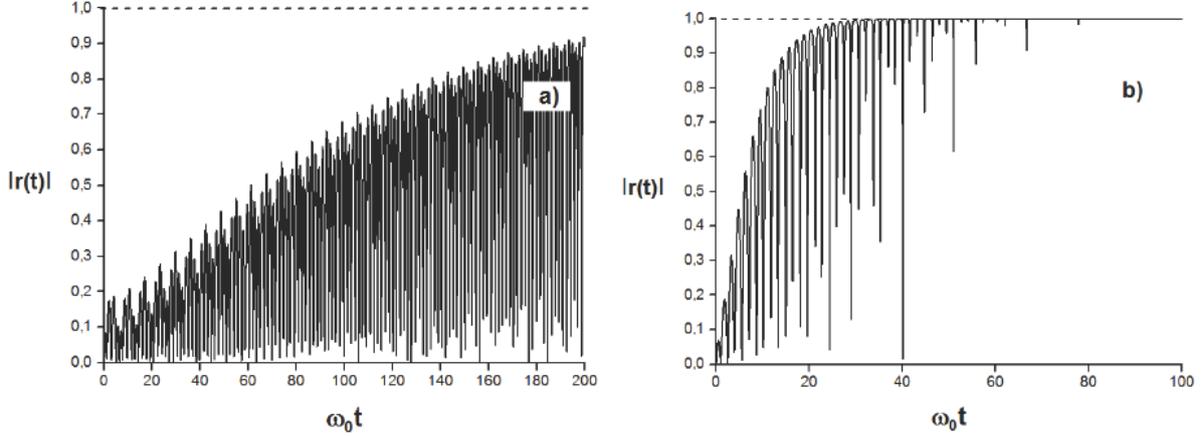


Figure 2. Correlation coefficient vs. time of action of the harmonic modulation of the well width given by eq. (10) at $g_{\Omega} = 0.1$ and two modulation frequencies: (a) $\Omega = \omega_0$ - resonant frequency, and (b) $\Omega = 2\omega_0$ - parametric resonance frequency [11].

Figure 2 shows evolution of the correlation coefficient in time under the action of the harmonic perturbation with frequencies $\Omega = \omega_0$ and $\Omega = 2\omega_0$ at $g_{\Omega} = 0.1$. Correlation coefficient oscillates with time but its amplitude $|r|_{\max}$ increases monotonously with the number of modulation cycles, $n = \omega_0 t / 2\pi$, resulting in a giant increase of the tunneling coefficient, as demonstrated in Fig. 3, which shows the TC evaluated by Eq. (10) that takes into account both the electron screening and the correlation effects [8]:

$$G^*(L, r) = \exp \left\{ - \frac{2\pi e^2}{\hbar_{\text{ef}}(r)} \sqrt{\frac{\mu}{2(E + e^2/L)}} \right\}, \quad (10)$$

where L is the minimum equilibrium spacing between D atoms determined by electron screening, E is their kinetic energy ($\sim eV/40$ at room temperature) \ll screening energy $\sim e^2/L$. One can see that the difference in electron screening and the corresponding initial D–D distances in a D_2 molecule ($L_0 = 0.74 \text{ \AA}$) and in the PdD crystal ($L_0 = 2.9 \text{ \AA}$) leads to a huge tunneling difference in the initial (uncorrelated) state, in which TC is negligible in both cases. However, with increasing number of modulation cycles, $\hbar_{\text{ef}}(r)$ increases according to Fig. 2 resulting in a giant increase of TC up to ~ 1 in several hundreds of cycles for $\Omega = \omega_0$ and in several dozens of cycles for parametric formation $\Omega \approx 2\omega_0$, which is more realistic to attain since it does not require exact coincidence of the frequencies [11].

The most important and nontrivial practical question now is how to realize such periodic action on an atomic scale? Modulation of the frequency of the optical phonon modes via excitation of the surface electron plasmons by a terahertz laser suggested in Ref. [11] as a driving force for the CCS formation is very questionable [8], and it does not explain LENR observed in the absence of the laser driving. In Section 3, we will consider a mechanism based on the large-amplitude time-periodic oscillations of atoms, which is an inherent LAV property.

3. LAV-induced Time-periodic Action on the Potential Barrier

3.1. Discrete breathers in bulk periodic crystals

The first attempts to develop a LENR mechanism in metal hydrides/deuterides (e.g. PdD or NiH) [8] were based on their crystal *periodic* structure, characteristic for *bulk* specimens or large particles. At ambient conditions, Pd

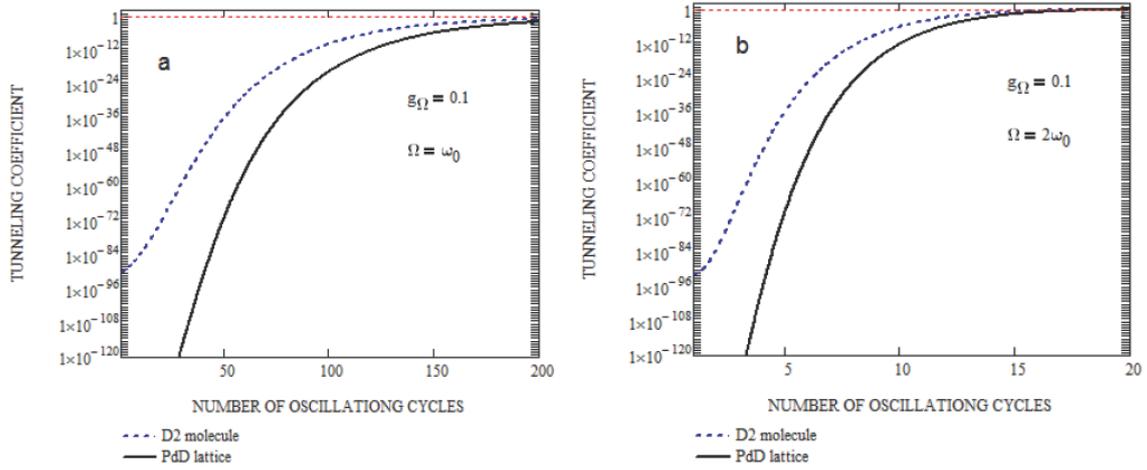


Figure 3. Tunneling coefficient increase with increasing number of the well modulation cycles, $n = \omega_0 t / 2\pi$, evaluated by Eq. (10) for $\Omega = \omega_0$ (a); $\Omega \approx 2\omega_0$ (b), $g_\Omega = 0.1$ for two D–D equilibrium spacings: in a D₂ molecule ($L_0 = 0.74 \text{ \AA}$) and in the PdD crystal ($L_0 = a_{\text{PdD}}\sqrt{2}/2 \approx 2.9 \text{ \AA}$). $a_{\text{PdD}} = 4.052 \text{ \AA}$ is the PdD lattice constant at 295 K [8].

hydrides/deuterides crystallize in FCC structure with the space group of the Rock-salt [21], while Pd hydrides/deuterides crystallize in various structures corresponding to NiH, NiH₂ and NiH₃ [22]. Molecular dynamic (MD) simulations have revealed that diatomic crystals with Morse interatomic interactions typically demonstrate *soft type* anharmonicity [23], which means that DB's frequency *decreases* with increasing amplitude, and one can expect to find so-called gap DBs with frequencies within the phonon gap of the crystal. The large mass difference between H or D and the metal atoms is expected to provide a wide gap in the phonon spectrum, in which DBs can be excited either by *thermal fluctuations* at elevated temperatures (as demonstrated for the different weight ratios and temperatures [24]), or by some *external driving* providing a sufficiently large initial displacement of a light atom from its equilibrium position (Fig. 4).

Thus, the D–D fusion rate in *bulk* PdD should be determined by the generation rate of DBs having amplitudes near the critical value $\sim 0.3 \text{ \AA}$, which has been evaluated in [8] for typical LENR conditions, resulting in a qualitative and quantitative agreement with experimental data on the fusion rate under D₂O electrolysis at the fitted set of well-defined material parameters (Fig. 5a). In particular, the model explains the crucial role of electric current under electrolysis that produces the flux of energetic deuterons (in the eV range) through the cathode surface, which is a driving force for the DB generation. In the absence of electric current, the LENR rate is predicted to be lower by five orders of magnitude (Fig. 5b).

With increasing temperature, the concentration of DB increases, resulting in increased power generation, in a *qualitative agreement* with experiments [14] (Fig. 5b). However, the model predicts much more powerful LENR output above 600°C than what is observed in Ni–H reactions [14]. This discrepancy appears because the model [8] did not take into account effect of *temperature fluctuations* on the tunneling efficiency of DBs. As has been shown by Vysotskii et al. [26], fluctuations interfere with formation of CCS, which means that the *temperature effect is two-fold and controversial*. On the one side, heating helps to excite DBs but on the other hand, it decreases their tunneling efficiency. Therefore, the best way to facilitate LENR, according to the present concept, is to look for an environment which favors formation of DBs (or, more generally, LAVs) at lower temperatures than those explored in typical LENR

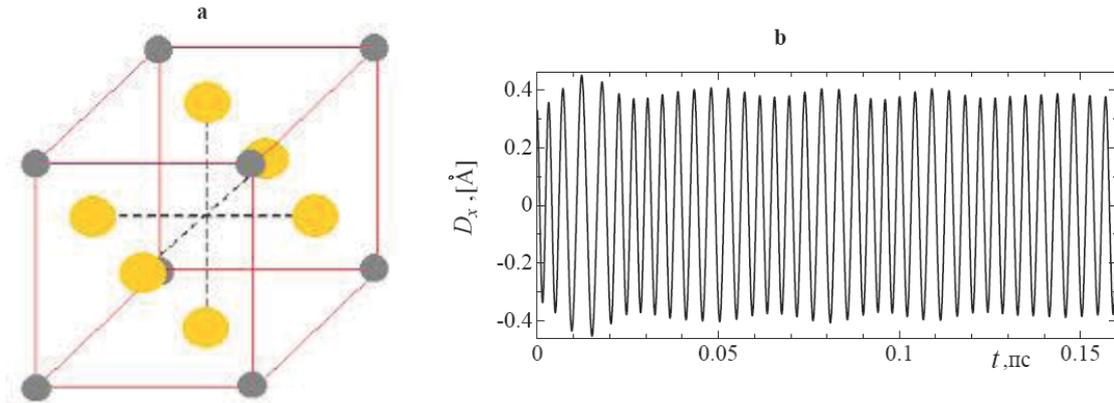


Figure 4. (a) A_3B compound based on FCC lattice with Morse interatomic potentials. Grey atoms are 50 times lighter than yellow ones. (b) DB initiated at zero Kelvin by the initial displacement $D_{x_0} \sim 0.3 \text{ \AA}$ of a light atom from its equilibrium position. It is localized on a *single light atom* vibrating along $\langle 100 \rangle$ direction with the frequency of 227 THz, which lies *inside the phonon gap*. Shown is the x -displacement of the light atom as the function of time. DB has a large amplitude of $\sim 0.4 \text{ \AA}$ that should be compared to the lattice parameter of 1.35 \AA [25].

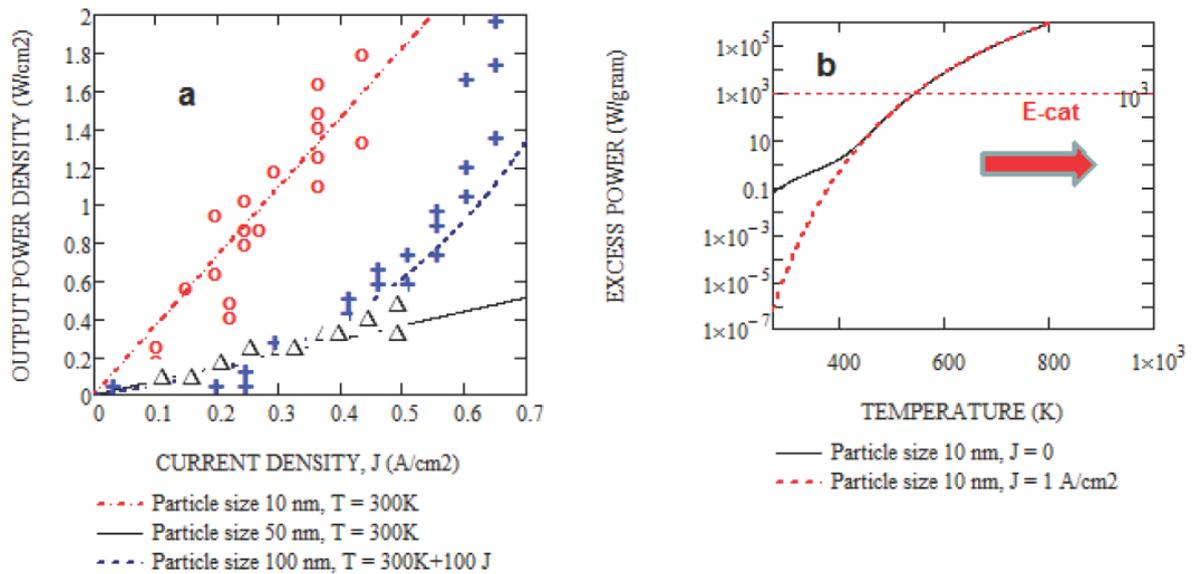


Figure 5. (a) LENR output power density according to the model in [8] vs. experimental data [13] as a function of electric current density at constant T and at T increasing with J as $T = 300 \text{ K} + 100 \text{ J}$. (b) LENR output power density according to the model [8] vs. temperature (broken line shows the power generation level in Ni–H reactions [14]).

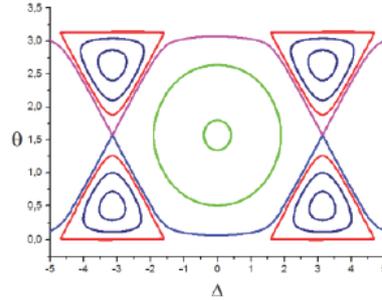


Figure 6. Phase diagram of two coupled anharmonic oscillators, according to the Ovchinnikov model [27] (see text). Separate regions in the diagram correspond to phase trajectories of the oscillators that *cannot share energy* [20].

installations. In Section 3.2, we consider LAVs in metal hydride/deuteride nanocrystals.

3.2. LAVs in nanocrystals and quasicrystals

The fact that the energy localization manifested by LAV does not require long-range order was first realized as early as 1969 by Alexander Ovchinnikov who discovered that localized long-lived molecular vibrational states may exist already in simple molecular crystals (H_2 , O_2 , N_2 , NO , CO) [27]. He realized also that stabilization of such excitations was connected with the *anharmonicity* of the intramolecular vibrations. Two coupled anharmonic oscillators described by a simple set of dynamic equations demonstrate this idea:

$$\begin{aligned}\ddot{x}_1 + \omega_0^2 x_1 + \varepsilon \lambda x_1^3 &= \varepsilon \beta x_2, \\ \ddot{x}_2 + \omega_0^2 x_2 + \varepsilon \lambda x_2^3 &= \varepsilon \beta x_1,\end{aligned}\quad (11)$$

where x_1 and x_2 are the coordinates of the first and second oscillator, ω_0 are their zero-point vibrational frequencies, ε is a small parameter, λ, β are the parameters characterizing the *anharmonicity* and the *coupling* force of the two oscillators, respectively. If one oscillator is displaced from the equilibrium and start oscillating with an initial amplitude, A , then the time needed for its energy to transfer to another oscillator is given by the integral:

$$T = \frac{\omega_0}{\varepsilon \beta} \int_0^{\pi/2} \frac{d\phi}{\sqrt{1 - (A^2 \gamma / 4)^2 \sin^2 \phi}}, \quad \gamma = \frac{3\lambda}{\beta}, \quad (12)$$

from which it follows that the full exchange of energy between the two oscillators is possible only at sufficiently small initial amplitude: $A^2 \gamma / 4 < 1$. In the opposite case, $A^2 \gamma / 4 > 1$, the energy of the first oscillator will *always be larger* than that of the second one. And for sufficiently large initial amplitude, $A \gg \sqrt{4/\gamma}$, there will be practically no sharing of energy, which will be localized exclusively on the first oscillator. This remarkable and seemingly *contra-intuitive* result is illustrated in Fig. 6 that shows the phase diagram of two coupled anharmonic oscillators.

Thus, Ovchinnikov has proposed the idea of LAV for molecular crystals, which was developed further for any nonlinear systems possessing *translational symmetry*; in the latter case, LAVs have been named *discrete breathers* (DBs) [6]^a or *intrinsic localized modes* (ILMs) [7]. Now, we are coming back to the idea of LAV arising at ‘*active*

^aNote that the term *discrete breathers* was coined nearly 20 years ago [6] in western nonlinear community, contrary to the recent comments [28] assigning the term to Ukrainian literature, while in the present paper we introduce a new and more general term ‘LAV’.

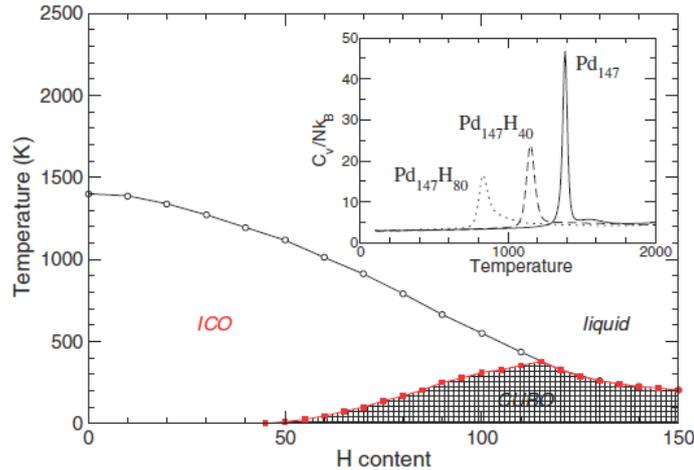


Figure 7. Schematic structural diagram of the $\text{Pd}_{147}\text{H}_x$ cluster in the icosahedral, cuboctahedral and liquid phases, after [32]. Inset: heat capacities of three clusters, in units of k_B per atom, versus canonical temperature. Icosahedral phase is predicted to be more stable above room temperature.

sites' in crystal defects, quasicrystals and nanoclusters. As noted by Storms [13], 'Cracks and small particles are the Yin and Yang of the cold fusion environment'. A physical reason behind this phenomenology is that in topologically disordered systems, sites are not equivalent and band-edge phonon modes are intrinsically localized in space. Hence, different families of LAV may exist, localized at different sites and approaching different edge normal modes for vanishing amplitudes [5]. Thus, in contrast to perfect crystals, which produce DB homogeneously, there is a striking *site selectiveness* of energy localization in the presence of spatial disorder, which has been demonstrated by means of atomistic simulations in biopolymers [5], metal nanoparticles [29] and, *experimentally*, in a decagonal *quasicrystal* $\text{Al}_{72}\text{Ni}_{20}\text{Co}_8$ [9]. In the latter case, the authors measured a so-called Debye–Waller factor defined by the mean-square thermal vibration amplitude of the atoms, and demonstrated that the anharmonic contribution to Debye–Waller factor increased with temperature much stronger than the harmonic (phonon) one. This was the first *direct observation* of a 'local thermal vibration anomaly', i.e. LAV, in our terms. The experimentally measured separation between LAVs was about 2 nm, which meant that their mean concentration was about 10^{20} per cm^3 that is many orders of magnitude higher than one could expect to find in periodic crystals [8].

The crystal shape of the nanoparticles (cuboctahedral or icosahedral) is known to affect their catalytic strength [30], and the possibility to control the shape of the nanoparticles using the amount of hydrogen gas has been demonstrated both experimentally by Pundt et al. [31], and by means of atomistic simulations by Calvo et al. [32]. They demonstrated that above room temperature the *icosahedral phase* should remain stable due to its higher entropy with respect to cuboctahedron (Fig. 7). And icosahedral structure is one of the forms quasicrystals take, therefore one is tempted to explore further the *link between nanoclusters and quasicrystals*.

Figure 8 shows the structure of $\text{Pd}_{147}\text{H}_{138}$ cluster containing 147 Pd and 138 H atoms having minimum free energy configuration, replicated using the method and parameters by Calvo et al. [32]. In particular, Fig. 8b reveals the presence of H–H–H chains aligned along the *I*-axis of the cluster. This *ab initio* simulation points out at the possibility of excitation of LAVs in these chains, with a central atom performing large-amplitude anharmonic oscillations and its neighbors oscillating in quasi-harmonic regime [34], which is similar to that considered in [8] for regular diatomic lattice of NaCl type. Such oscillations have been shown to stimulate formation of CCSs [8] and to facilitate LENR. In

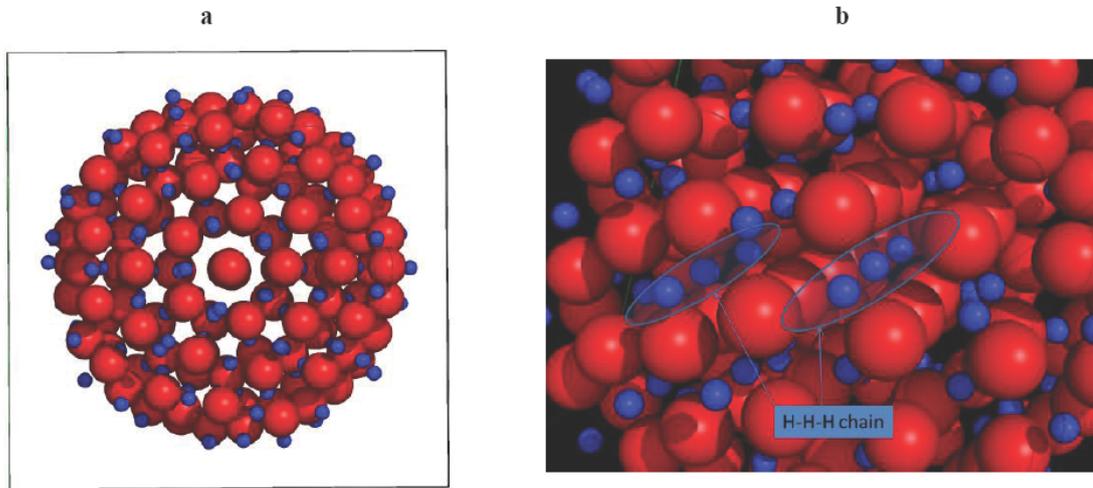


Figure 8. (a) Structure of PdH cluster containing 147 Pd and 138 H atoms having minimum free energy configuration, replicated in [33] using the method and parameters by Calvo et al. [32]; (b) H–H–H chains in the nanocluster, which are viable sites for LAV excitation [34].

Section 4, we will consider the ways of excitation of LAVs based on the present concept.

4. Ways of LAV-LENR Triggering

The main message of this paper is that the excitation of LAVs present an efficient way to produce CCS due to time-periodic modulation of the potential well width (or the Coulomb barrier width) and hence to trigger LENR in solids. As has been mentioned above, heating helps to excite LAVs but it decreases their tunneling efficiency. Therefore, we need ways to excite LAVs at sufficiently low temperatures, which is not a trivial problem technically.

One of the methods is based on time-periodic shaking of the surface atoms at frequencies near the optic phonon edge resulting in the LAV excitation in the sub-surface layers. Medvedev et al. [35] has demonstrated by means of MD simulations that gap DBs can be excited in the Al sub-lattice of Pt_3Al under the action of *time-periodic external driving*. Time-periodic shaking of the surface atoms at frequencies near the optic phonon edge resulted in the DB excitation in the sub-surface layers. These findings point out at the possibility of LENR stimulation by external time-periodic excitation of surface atoms. This method has been actually realized in terahertz laser experiments [36] on the stimulation of LENR by a joint action of two low-power laser beams with variable beat frequency ranging from 3 to 24 THz on the cathode surface during the D_2O electrolysis in the PdD system.

Figure 9 shows the experimental frequency dependencies of the excess power in these experiments. Three main resonances of excess energy released at $\sim 8 \pm 1$ THz, 15 ± 1 THz and 21 ± 1 THz have been shown in [8] to correlate with the DB-induced harmonic frequency, $\omega_0 (A_{\text{cr}}) \approx 7.5$ THz, DB parametric frequency $\Omega (A_{\text{cr}}) \approx 15$ THz and DB initial frequency, 21 THz, respectively. According to the model in Ref. [8], the highest resonance is the biggest, since it is caused by amplification of DB excitation at the edge of optic phonon band. The medium resonance is due to tuning action of external driving on the DB frequencies: it increases the fraction of DBs with parametric frequency. The lowest resonance is due to tuning of harmonic frequencies by external driving: it increases the fraction of D atoms subjected to the parametric action by DBs.

The atoms are shaken by laser beams via excitation of the surface electron plasmons as suggested in [36]. It

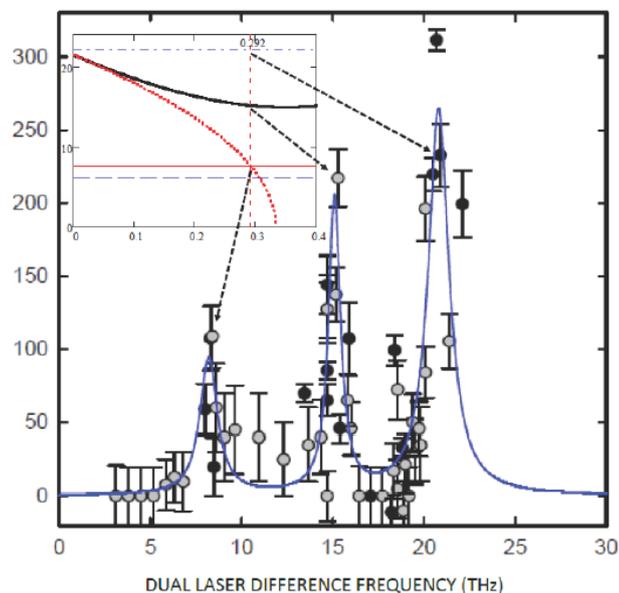


Figure 9. Excess power (mW) under joint action of two low-power laser beams with variable beat frequency on the surface of the Pd cathode during the electrolysis in heavy water [36]. The inset (from [8]) shows parity between critical DB-induced frequencies and the resonance frequencies [36] designated by dashed arrows.

explains the necessity of external magnetic field for producing resonance effects. However, the direct modulation of the frequency of the optical phonon modes by plasmons proposed in [11] as a driving force for the CCS formation is very questionable [8], and it does not explain LENR *observed in the absence of the laser driving* at slightly higher electric current or temperatures [36]. In the present view, the laser driving acts only as a tuning tool for the CCS formation by DBs induced in this case by joint action of temperature and electric current. Therefore, in order to stimulate LENR, one needs to apply some external triggering of LAVs similar to that provided by electric current under electrolysis conditions (below 100°C). Some phenomenological attempts to generate such triggering are currently underway [37,38], but the frequency range used in such attempts is far away from the LAV frequencies lying typically in THz diapason. These experiments did not show any evidence of excess heat within the accuracy of measurements. In the present view, this frequency mismatch may be responsible for the inefficiency of such triggering, which shows the need for a *physically based* frequency range and other methods of the LAV-LENR triggering.

From the experiments [36] on the resonant enhancement of excess heat generation by dual laser beams, one may conclude that the required frequency range lies in the terahertz diapason (8–20 THz in the Pd–D system). However, the exact value of the frequency required to trigger LAV-LENR in the Ni–H system *is not known* at present, and if the irradiation frequency does not match the LAV frequency, no effect is expected, in contrast to simple heating that excites all phonon modes. Therefore, the *first practical suggestion* of the LAV-concept is that one needs a laser with *variable frequency* in the THz range in order to fit the required frequency *in situ* experiments and trigger LENR.

The second suggestion is that instead of *heating*, which decreases the LAV efficiency, a *cooling* of the nuclear ‘fuel’ may result in the enhancement of the LENR output. This idea is illustrated in Fig. 10 which shows that the wave lengths corresponding to the desired frequency range (e.g. 6–30 THz) lie in the deep infrared diapason (10–50 μm),

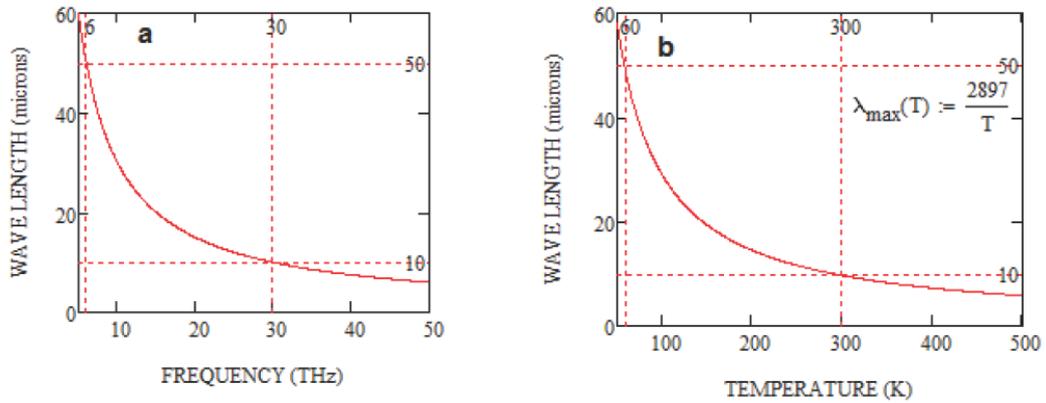


Figure 10. Wave length vs. frequency (a) and the maximum wave length vs. temperature of black body (b) according to Wien's law (1893).

which is emitted by a black body having temperature ranging from the room temperature down to liquid nitrogen temperature (Fig. 10b).

Thus, a combination of appropriate triggering with cooling may result in the extremely cold fusion and other

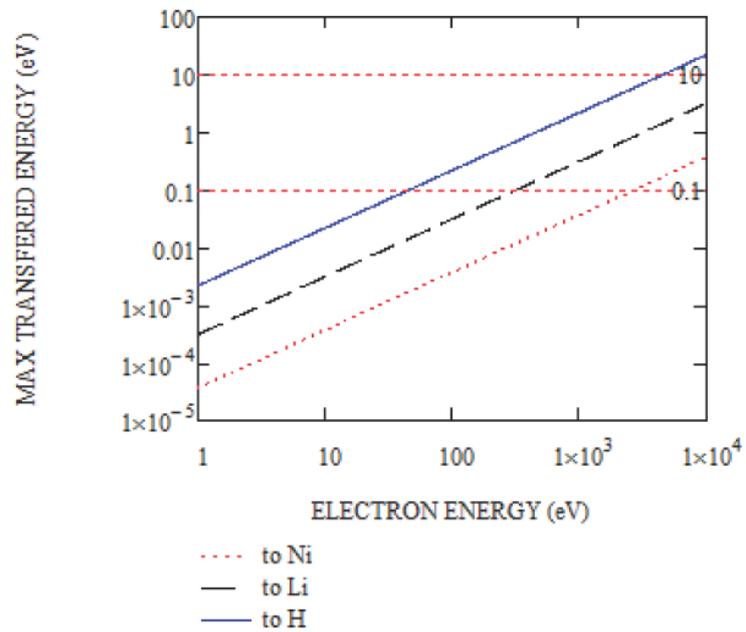


Figure 11. Maximum transferred energy of electrons to the target atoms (Ni_{58} , Li_7 and H_1) vs. the electron energy.

nuclear reactions in a nuclear active environment enriched with potential LAV sites.

5. Experimental Verification

As mentioned above [37,38], a majority of attempts to replicate the Ni–H LENR failed, which has led J.P. Biberian to the following conclusion [37]: “Reproducing Rossi’s experiment following Parkhomov’s process is not as easy as it seemed. After more than 20 experiments with nickel and LiAlH_4 in different configurations, within the precision of the calorimeter of ± 2 W, no excess heat was measured.”

However, there have been several successful LENR replications reviewed by Parkhomov [39,40], where the excess energy production in Ni–H has been observed in amounts exceeding those expected from chemical reactions. This controversy of different experimental results points out to the necessity of careful *examination and comparison of microstructures* of successful and unsuccessful fuels, and to the need to search the *new ways of triggering LENR*, which could result in a higher success rate.

One of the perspective ways of triggering LENR is to use *electron beams*. The point is that electrons hitting the target atoms displace them from equilibrium positions by a distance depending on the electron energy and the atomic mass. The displaced atoms start vibrating with frequencies inversely proportional to the initial displacements. If the frequency (i.e. initial displacement) matches the LAV frequency, a LAV is generated.

Figure 11 shows the dependence of the maximum transferred energy of electrons to the target atoms on the beam energy. It can be seen that in order to transfer energy between 0.1 and 10 eV to the light atoms H_1 or Li_7 (required to excite LAV) one needs electrons of keV energy range. It means that one needs a technology allowing electrons with keV energy range to interact with atoms inside the Ni–Li–H ‘fuel’ in order to catalyze LENR. However, *the problem* is that electrons of keV energies can penetrate only a few sub-surface atomic layers due to a strong scattering by the lattice, and hence, an *external electron beam* can excite only a thin surface layer. Dubinko [41] proposed a solution to this problem by using *Bremsstrahlung* gamma and *Characteristic X-rays* produced by accelerated electrons hitting a metallic converter and atoms of the fuel mixture.

For example, a tantalum converter has a characteristic tantalum peak at ~ 60 keV and another peak at ~ 150 keV. These gammas can penetrate up to a range centimeters deep, and they are absorbed by the Compton mechanism, which transforms them into electrons and gammas of lower energy *inside the fuel mixture*. Gammas with energies below 100 keV are converted *inside the fuel mixture* into electrons of the same energies due to the photoelectric effect. A part of resulting electrons will scatter at the fuel atoms elastically resulting in the energy transfer to them and hence to their displacement from equilibrium positions. Another part of electrons will produce characteristic X-rays inside the fuel mixture with energies determined by the fuel elements. For example nickel and aluminum will produce X-rays of ~ 8 and ~ 1.5 keV, respectively, which will be again converted to electrons of the same energies *inside the fuel mixture* by photoelectric effect. In this way, atoms entering the fuel mixture will be ‘kicked’ away from their equilibrium positions by electrons of different energies with local *Characteristic peaks* determined by the elements of the fuel. Adding various elements into the fuel mixture, it may be possible to change the energy spectrum of the ‘kicks’ and fit the required composition for the most effective *homogeneous* excitation of LAV in the fuel bulk, resulting in the LENR catalysis.

6. Conclusions and Outlook

In the present paper we argue that the excitation of LAVs presents an efficient way to produce CCS due to time-periodic modulation of the potential well width (or the Coulomb barrier width) and hence to trigger LENR in solids. This *LAV concept* is a natural extension of the breather nano-collider (*BNC*) concept proposed in [8]. In its initial form [8], it did not take into account quantum correlation effects, and hence, unrealistically small separation between atoms

($\sim 0.01 \text{ \AA}$) would have to be attained in order to enhance the LENR rate up to a noticeable level. Accounting for the correlation effects (Dubinko 2015) has shown that the *oscillation amplitude of several fractions of an angstrom* may be sufficient to produce the required effect, if CCS parametric conditions are met. Recent results obtained by a direct numerical solution of the time-dependent Schrödinger equation for a single nuclear particle in a harmonic [28] and double well potential [42] confirmed this view. It has been shown that these oscillations of the well width will periodically delocalize the nucleus and facilitate the tunneling of adjacent nuclei into the Strong Force attractive nuclear potential well, giving rise to nuclear fusion at rates that are *several tens of orders of magnitude* larger than what one calculates with the usual Gamow Factor integral relationship.

One of the important practical considerations following from the breather-induced correlation effects is that the breather *lifetime* plays more important role than the minimum distance between the oscillating nuclei.

Another critical parameter is the *mean concentration* of the CCS produced by the oscillations. In the present paper we extended the concept of *DBs* arising in perfect crystals homogeneously, to the *LAVs* that showed a striking *site selectiveness* of energy localization in the presence of spatial disorder, which has been demonstrated by means of atomistic simulations in biopolymers [5], metal nanoparticles [29] and, *experimentally*, in some quasicrystals [9]. The experimentally measured concentration of *LAVs* in the latter amounts to $\sim 10^{20}$ per cm^3 , which is many orders of magnitude higher than one could expect to find in periodic crystals [8].

Analysis of the *LAV* frequency range suggests that instead of the currently explored *heating*, which decreases the *LAV* tunneling efficiency, a *cooling* of the nuclear ‘fuel’ may result in the enhancement of the LENR output, provided that it is combined with an appropriate *triggering* of the *LAV* formation by a special *electro-magnetic or electron* irradiation.

In conclusion, we note that the present concept is based only on the *known physical principles* and on independent atomistic simulations of *LAVs* in crystals using realistic many-body interatomic potentials and on the *ab initio* simulations of the structure of Me–H clusters. Atomistic modeling of *LAVs* of various types in metal hydrides/deuterides is an important outstanding problem since it may offer ways of *engineering the nuclear active environment* and help to discover the frequency/amplitude range of *LAVs* required for LENR triggering.

Acknowledgements

The author would like to thank Denis Laptev for designing Figs. 1,2 and 6; Sergey Dmitriev for Fig. 4; Dmitry Terentyev for Fig. 8, and Dan Woolridge for the *LAV* animation [34]. I thank Klee Irvin for attracting my attention to the new and promising field of quasicrystal research. Financial support from Quantum Gravity Research is gratefully acknowledged.

References

- [1] G. Ertl, H. Knozinger, F. Schuth, F., J. Weitkamp (Eds.), *Handbook of Heterogeneous Catalysis*, 2nd edn, Wiley-VCH, 2008.
- [2] R.S. Swathi and K.L. Sebastian, Molecular mechanism of heterogeneous catalysis, *Resonance* **13**(6) (2008) 548–560.
- [3] M. Yoshimura and A.P. Tsai, Quasicrystal application on catalyst, *J. Alloys and Compounds* **342** (2002) 451–454.
- [4] V.I. Dubinko, P.A. Selyshchev and J.F.R. Archilla, Reaction-rate theory with account of the crystal anharmonicity, *Phys. Rev. E* **83**(4) (2011) 041124.
- [5] F. Piazza and Y.H. Sanejouand, Discrete breathers in protein structures, *Phys. Biol.* **5** (2008) 026001; V.I. Dubinko and F. Piazza, On the role of disorder in catalysis driven by discrete breathers, *Lett. Materials* **4** (2014) 273. <http://lettersonmaterials.com/en/Readers/Article.aspx?aid= 712>.
- [6] S. Flach and A.V. Gorbach, Discrete breathers, *Phys. Rep.* **295** (1998) 181–264.
- [7] V. Hizhnyakov, M. Haas, A. Shelkan and M. Klopov, Theory and molecular dynamics simulations of intrinsic localized modes and defect formation in solids, *Phys. Scr.* **89** (2014) 044003-1-5.

- [8] V.I. Dubinko, Low-energy Nuclear reactions driven by discrete breathers, *J. Condensed Matter Nucl. Sci.* **14** (2014) 87–107, V.I. Dubinko, Quantum tunneling in gap discrete breathers, *Lett. Materials* **5** (2015) 97–104. <http://lettersonmaterials.com/en/Readers/Article.aspx?aid=810>; Vladimir Dubinko, Quantum Tunneling in Breather ‘Nano-colliders’, <http://www.lenr-forum.com/forum/index.php/Thread/1014-Breather-Nano-Collider-for-LENR-explanation/?postID=4300#post4300>.
- [9] E. Abe, S.J. Pennycook and A.P. Tsai, Direct observation of a local thermal vibration anomaly in a quasicrystal, *Nature* (London) **421** (2003) 347–350.
- [10] V.V. Dodonov and V.I. Man’ko, *Phys. Lett. A* **79**(2/3) (1980) 150.
- [11] V.I. Vysotskii and M.V. Vysotskiy, *Euro. Phys. J. A* **49** (2013) 99, DOI 10.1140/epja/i2013-13099-2.
- [12] M. McKubre, F. Tanzella, P. Hagelstein, K. Mullican and M. Trevithick, The need for triggering in cold fusion reactions, in *Tenth Int. Conf. on Cold Fusion*, MA, LENR-CANR.org., Cambridge, 2003.
- [13] E.K. Storms, *The Science of Low Energy Nuclear Reaction*, World Scientific, Singapore, 2007.
- [14] A.G. Parkhomov, *Int. J. Unconventional Sci.* **7**(3) (2015) 68.
- [15] H.J. Assenbaum, K. Langanke and C. Rolfs, *Z. Phys. A* **327** (1987) 461.
- [16] J. Kasagi, Screening potential for nuclear reactions in condensed matter, in *ICCF-14, Int. Conf. on Condensed Matter Nucl. Sci.*, 2008.
- [17] E. Schrödinger, *Ber. Kgl. Akad. Wiss., Berlin, S.* **24** (1930) 296.
- [18] H.P. Robertson, *Phys. Rev.* **34** (1930) 163.
- [19] V.V. Dodonov and V.I. Man’ko, Invariants and evolution of nonstationary quantum systems, *Proc. Lebedev Physics Institute*, Vol. 183, M.A. Markov (Ed.), Commack, Nova Science, New York, 1989.
- [20] V.I. Dubinko and D.V. Laptev, Chemical and nuclear catalysis driven by localized anharmonic vibrations, *Lett. Materials* **6** (2016) 16–21.
- [21] I. Errea, M. Calandra1 and F. Mauri, First-principles theory of anharmonicity and the inverse isotope effect in superconducting palladium-hydride compounds, *Phys. Rev. Lett.* **111** (2013) 177002.
- [22] S. Kanagaprabha, A. Meenaatci, R. Rajeswarapalanichamy and K. Iyakutti, First principles study of electronic structure, structural properties and superconductivity of nickel hydride, *Walailak J. Sci. Technol.* **9**(2) (2012) 115.
- [23] L.Z. Khadeeva and S.V. Dmitriev, Discrete breathers in crystals with NaCl structure, *Phys. Rev. B* **81** (2010) 214306 (8 pp).
- [24] L.Z. Khadeeva and S.V. Dmitriev, Lifetime of gap discrete breathers in diatomic crystals at thermal equilibrium, *Phys. Rev. B* **84** (2011) 144304 (8 pp).
- [25] S.V. Dmitriev, *Private communication*.
- [26] V.I. Vysotskii, S.V. Adamenko and M.V. Vysotskiy, Formation of correlated states and increase of the barrier transparency for low energy particles in nonstationary systems with damping and fluctuations, *J. Exp. Theoret. Phys.* **142** (2012) 627–643.
- [27] A.A. Ovchinnikov, Localized long-lived vibrational states in molecular crystals, *Zh. Eksp. Teoret. Fiz.* **57** (1969) 2137, *Sov. Phys. JETP.* **30** (1970) 116.
- [28] Louis DeChiaro, <http://www.e-catworld.com/2015/10/06/louis-dechario-of-us-naval-sea-systems-command-navsea-on-replicating-pons-and-fleischmann/>.
- [29] H. Zhang and J.F. Douglas, Glassy interfacial dynamics of Ni nanoparticles: Part II Discrete breathers as an explanation of two-level energy fluctuations, *Soft Matter* **9** (2013) 1266–1280.
- [30] *Metal Nanoclusters in Catalysis and Materials Science: The Issue of Size Control* (Eds.) B. Corain, G. Schmid, N. Toshima, 2008.
- [31] A. Pundt, A. Dornheim, M. Guerdane, H. Teichler, H. Ehrenberg, M.T. Reetz and N.M. Jisrawi, Evidence for a cubic-to-icosahedral transition of quasi-free Pd–H-clusters controlled by the hydrogen content, *Euro. Phys. J. D* **19** (2002) 333. (doi:10.1140/epjd/e20020080).
- [32] F. Calvo and A. Carré, Structural transitions and stabilization of palladium nanoparticles upon hydrogenation, *Nanotechnology* **17** (2006)1292–1299.
- [33] V. Dubinko and D. Terentyev, Molecular dynamic simulation of localized anharmonic vibrations in metal-hydrogen nanocrystals, to be published.
- [34] D. Woolridge, *Quantum Gravity Research*, Los Angeles, CA 90290, USA, <https://www.dropbox.com/s/557akac5zoynqs/LAV%20animation%20in%20PdH%20cluster.mp4?dl=0>

- [35] N.N. Medvedev, M.D. Starostenkov, P.V. Zakharov and O.V. Pozhydaeva, *J. Tech. Phys. Lett.* **37** (2011) 7.
- [36] D. Letts and P.L. Hagelstein, Stimulation of optical phonons in deuterated palladium, in ICCF-14, *Int. Conf. on Condensed Matter Nucl. Sci.*, Washington, DC, 2008; P.L. Hagelstein, D. Letts and D. Cravens, Terahertz difference frequency response of PDD in two-laser experiments, *J. Condensed Matter Nucl. Sci.* **3** (2010) 59–76.
- [37] Jean-Paul Biberian, Replication attempts of the Parkhomov experiment, *Proc. 11th Int. Workshop on Hydrogen Loaded Metals*, October 15–16, 2015.
- [38] K.P. Budko and A.I. Korshunov, Calorimetric investigation of anomalous heat production in Ni–H systems, *Proc. 11th Int. Workshop on Hydrogen Loaded Metals*, October 15–16, 2015.
- [39] A.G. Parkhomov, Ni–H reactors created after the Lugano Report, *Int. J. of Unconventional Sci.* **11**(4) (2016) 58. <http://www.unconv-science.org/n11/parkhomov/>.
- [40] A.G. Parkhomov, Long-term tests of Ni–H thermal generators in flow calorimeter, *Int. J. Unconventional Sci.* **12,13**(4) (2016) 74. <http://www.unconv-science.org/n12/parkhomov/>.
- [41] V.I. Dubinko, Radiation-induced catalysis of low energy nuclear reactions in solids, *J. Micromechanics and Mol. Phys.* **1** (2016) 165006-1-12.
- [42] V. Dubinko, D. Laptev and K. Irwin, Catalytic mechanism of LENR in quasicrystals based on localized anharmonic vibrations and phasons, presented at *ICCF20*, Sendai, October 2016, to be published in JCMNS.