

Research Article

Simulation of Crater Formation on LENR Cathodes Surfaces

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Abstract

Many authors reported the presence of small-size craters on the surface of cathodes after Low-energy Nuclear Reaction (LENR) electrolysis experiments. It is conjectured the craters result from violent reactions, perhaps of nuclear origin. Nagel proposed a correlation between the crater diameter and the energy involved in its formation. Starting from this assumption, it can be estimated that the enthalpy released can raise the temperature of the crater content to about 2000 K. A simple model is used to calculate the crater cooling by conduction and radiation. It gives the order of magnitude of the maximum event duration in order to achieve some melting of the cathode material. The duration of the eruption is estimated from the gas pressure developed within the crater. A value of 6 ns is obtained for a 2 μm diameter, and 600 ns for a 20 μm crater. In large craters, a part of inner material can be molten. Small craters are strongly cooled by the surrounding metal and do not show signs of fusion.

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1. Introduction

Several authors observed small-size craters on the surface of metals after electrolysis experiments. They have been reported on different metals, but mostly on palladium cathodes [1–5].

The morphology of these structures is very similar to the craters created by the impact of high-speed objects, like meteorites or bullets [6]. A round shaped void can be seen with the periphery protruding from the original surface. In the case considered here, the dimensions of the craters are small, in the range of a few micrometres to a few tens of micrometres.

The similarity of the shape of these craters with the large ones raises the question of the phenomenon responsible for their formation. It is tempting to assume that local reactions led to the melting and eruption. Elemental analysis in and near the craters suggests that the craters could mark the location of LENR events [2–5]. The relation between the presence of craters and excess heat is not yet fully established [6]. However, craters are frequently seen on cathodes, which gave excess heat. The simple fact that craters could be the sites of creation of at least a fraction of the LENR energy makes it interesting to further investigate the question of the energetics and dynamics of their formation.

This paper presents some estimations of the typical time scales involved for the different phenomena taking place during the formation of craters and discusses the main results.

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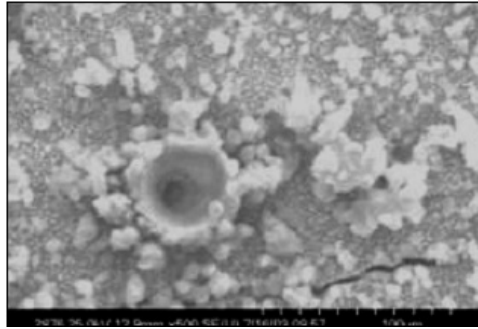


Figure 1. Large crater with a rounded shape. There are evident signs of melting of the ejected material, some of it solidified around the crater rim. The diameter is 50 μm . The original point of the explosion seems to be located several tens of μm below the surface [3].

2. Examples of Craters Observed on Palladium Cathodes of LENR Experiments

Nagel discussed the different types of craters observed [6]. The observed diameters are generally between 2 and 50 μm , and a few are larger. In most cases, the craters exhibit a circular shape. The ratio between the crater depth and diameter ranges between 0.5 and 5.

3. Energy of Crater Formation

Kim [7] calculated the energy required to melt or vaporize the quantity of metal located in a cone having the dimensions of the crater considered. For a crater with a diameter of 50 μm and a depth of 25 μm , the energy calculated is 3.2×10^{-5} J, if we consider that the metal is molten, or 6.5×10^{-4} J if the metal is vaporized. Assuming these energies result from D–D fusion into He^4 , they correspond respectively to 8.3×10^6 and 1.7×10^8 nuclear reactions.

Nagel [6] compared the dimensions of craters of very different origins and the energy involved for their formation. A simple correlation can be drawn between the size and the energy. The relationship obtained is reproduced in Fig. 5. Nagel compared the values given by Kim with his own investigations. The orders of magnitude agree quite well. The energy given by the correlation falls between the values calculated assuming melting and vaporization.

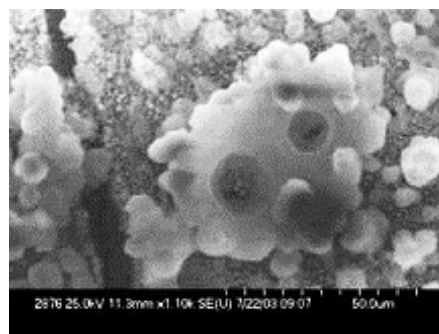


Figure 2. Two adjacent craters, 15 and 10 μm in diameter. The larger one is fully rounded, while a hexagonal shape can still be recognized in the small one. Although both embedded within a common mass of molten material, they do not seem to be obviously correlated [3].

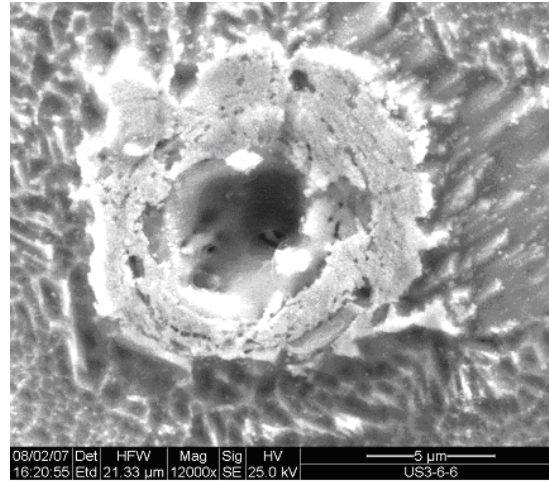


Figure 3. Micrograph showing a 6 μm diameter crater. One can notice the round shape, the concentric rings of ejected material and the deformation of the surrounding metal surface [5].

In the following, we assume that the energy required for cratering is given by the correlation of Fig. 5. The corresponding energy is 10^{-3} J for a crater 100 μm diameter and 50 μm deep, with a volume of $1.31 \times 10^5 \mu\text{m}^3$. The energy density is then $7.6 \times 10^9 \text{ J m}^{-3}$, or 640 kJ kg^{-1} . Accordingly, the correlation can be described by the equation:

$$E_i = \alpha_i \cdot V, \quad (1)$$

where E_i is the energy input (J), $\alpha_i = 7.6 \times 10^9 \text{ J m}^{-3}$ (equivalent to 640 kJ kg^{-1}) and V is the crater volume (m^3).

Figure 6 shows the relationship between the temperature and the specific enthalpy of palladium [8]. It can be seen that the enthalpy mentioned above corresponds to a temperature close to 2000 K.

4. Simple Modelling of the Main Phenomena

4.1. Basis of the simulation

The estimation of the energy does not give information about the kinetics of the crater formation. The simple model presented here gives some insight.

The only features, which can be observed, are the craters left after the eruption. The precise sequence of the phenomena cannot be directly observed, but can at most be derived from a simulation.

The only things known at the beginning are as follows:

- Craters are present on the surface, showing that some material is ejected away from the cathode.
- The largest craters have a circular shape and show signs of melting.
- The smallest ones may have a non-circular shape and do not exhibit traces of molten metal.
- According to Nagel and the discussion of the previous paragraph, the energy involved in the crater formation corresponds to the heating of a hot core up to 2000 K before the eruption.

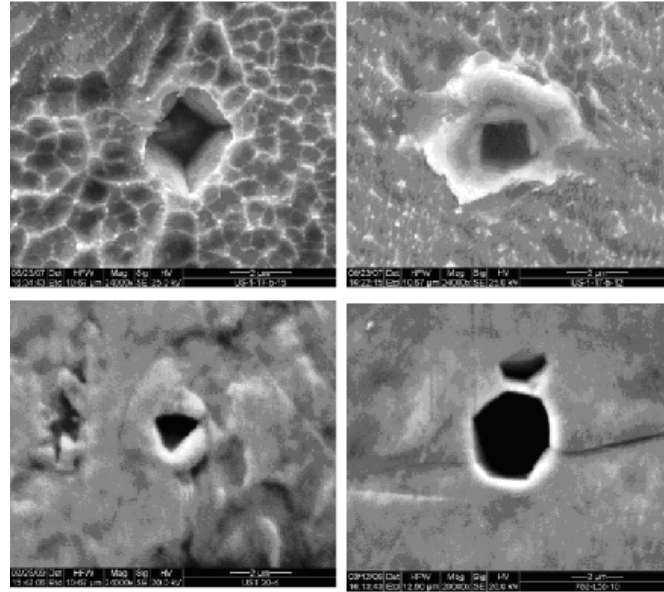


Figure 4. Micrographs of small craters from Super-wave experiments by M. Tsirlin . Published by Nagel [6]. The diameters range from 1 μm to 2 μm . There are no signs of melting. The shapes appear to be influenced by the cathode crystal structure.

The simulation must be able to explain these observations. We are going to follow three distinctive steps in order to introduce the main phenomena

- In the first step, we examine the temperature evolution of a hot core before the eruption. This will show that a hot core having small dimensions cools down very fast. The cooling time gives an upper bound of the possible LENR event duration.

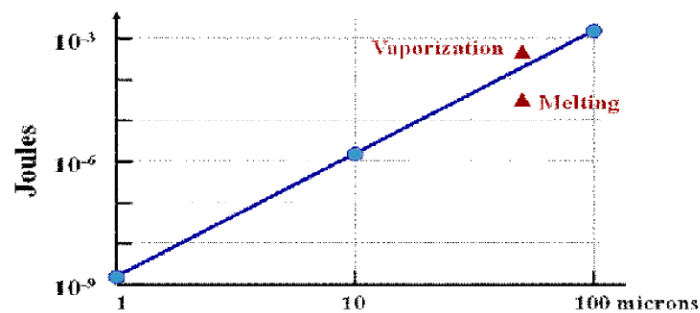


Figure 5. Correlation between the crater diameter and the energy necessary for its formation [6].

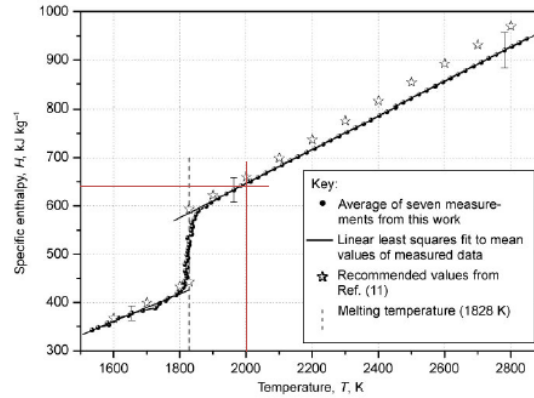


Figure 6. Specific enthalpy of palladium [8] The value α_i from Eq. (1) is indicated. It corresponds to a heating of the metal up to 2000 K.

- The dynamics of the eruption is evaluated. The comparison of the time required for the ejection of the crater content and of the cooling time explains why melting is only observed in large craters
- The fact that most craters are circular suggests that the initial LENR sites are smaller than the craters observed on the surface. The logical consequences of this last assumption are discussed.

At this stage, the model uses very rough assumptions. However, they are enough to find out the orders of magnitude of the different phenomena involved:

- (1) Thermal flow between the crater and the surrounding metal
- (2) Heat radiated out of the crater considered as a black body
- (3) Eruption and ejection of the crater content

4.2. Hot core cooling

A small volume with dimensions of a few micrometres cools down very fast. The purpose of the simulation is to obtain a quantitative figure of the duration during which a hot core can retain a high temperature. Obviously, the duration of the LENR event responsible for the formation of the hot core must be shorter than the cooling time, otherwise the energy is dissipated away while it is released by the LENR event and the hot core temperature remains limited.

4.2.1. Thermal flow by conduction

We assume that the energy input is supposed to be confined in a spherical core which has the same volume as the final crater. The energy is in the form of enthalpy within the material contained inside the crater just before the eruption and is given by Eq. (1). The heat is transferred to the surrounding metal by conduction.

In order to simplify the calculation, we consider in a first approach that the hot core is deeply embedded below the surface, as shown in Fig. 7. The reaction does not create a crater on the surface and cooling only results from conduction in the solid metal surrounding the hot core.

Hypotheses:

- The matrix is made of palladium.

Table 1. Palladium properties.

Density	12 023 kg m ⁻³
Melting	1555°C = 1828 K
Boiling	2963°C = 3236 K
Specific heat	245 J kg ⁻¹ K ⁻¹
Thermal conductivity	71 W m ⁻¹ K ⁻¹ at 20°C
Velocity of sound	3070 m s ⁻¹

- Before the reaction, the base metal is a solid body.
- The reaction takes place uniformly throughout the core, a sphere with a radius, R .
- No eruption takes place.
- The energy input E_i is proportional to the core volume, as per Eq. (1).
- The reaction evolves at a constant pace, during a reaction time τ . This duration is taken as a variable to study its influence.
- The energy is transferred by conduction.
- The heat capacity and the thermal conductivity are constant, taken for pure palladium

The last hypothesis neglects the fact that the metal is loaded with deuterium. This simplification is addressed below. It should not alter the orders of magnitude of the results.

The heat flow is computed according to a spherical model using the Fourier equation of heat conduction, see Fig. 8. Within the core with a radius R , some energy α_i is released per unit volume. It is assumed that this energy evolves at a constant pace during the reaction time τ . Between time $t = 0$ and time $t = \tau$ the reaction creates in the volume dV a local energy input dW :

$$\frac{dW}{dV} = \frac{\alpha_i}{\tau} dt. \quad (2)$$

The solid taken into account in the model has the properties of pure palladium, as listed in Table 1.

In fact, in LENR experiments, the palladium is loaded with deuterium, so that at least a part of the metal is transformed into hydride PdD_x. The values of x are larger than 0.6 and can be close to 1. The properties of the hydride differ from metallic Pd. In particular, the density is lower, about 10⁴ kg m⁻³. The other properties are not well known.

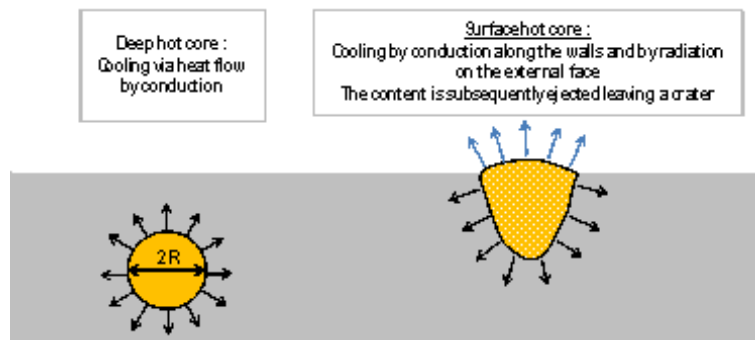


Figure 7. Schematic representation of hot core cooling – The hot core is the volume heated up to 2000 K by the LENR event – defined by Nagel's equation.

In any case, as only the orders of magnitude are calculated, the precise characteristics are not absolutely necessary at this stage, so that pure palladium properties are used for this first approach.

The results of the heat flow model are presented for two different core diameters: 2 and 20 μm . The energy inputs E_i are proportional to the volumes according to Eq. (1). They are, respectively, 2.12×10^{-8} and 2.12×10^{-5} J.

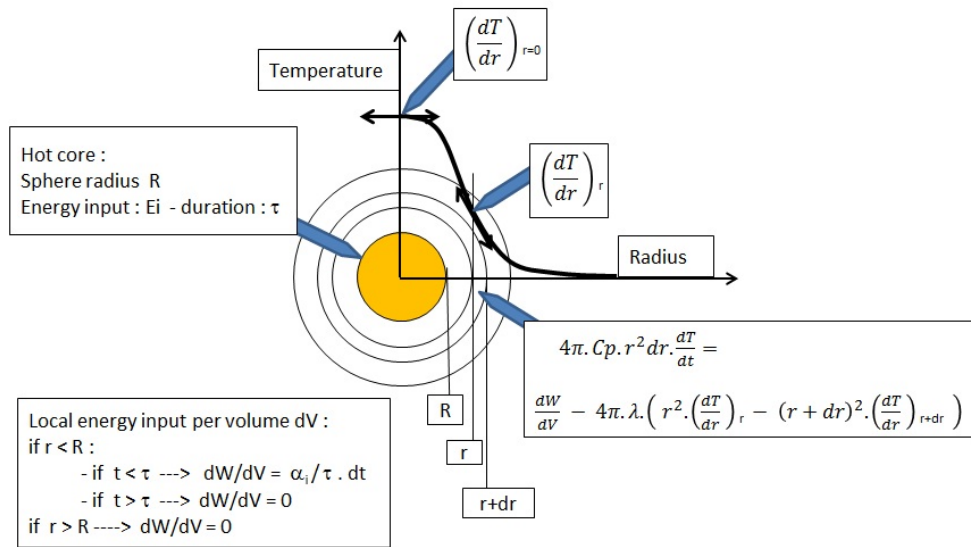


Figure 8. Schematic representation of the heat flow model.

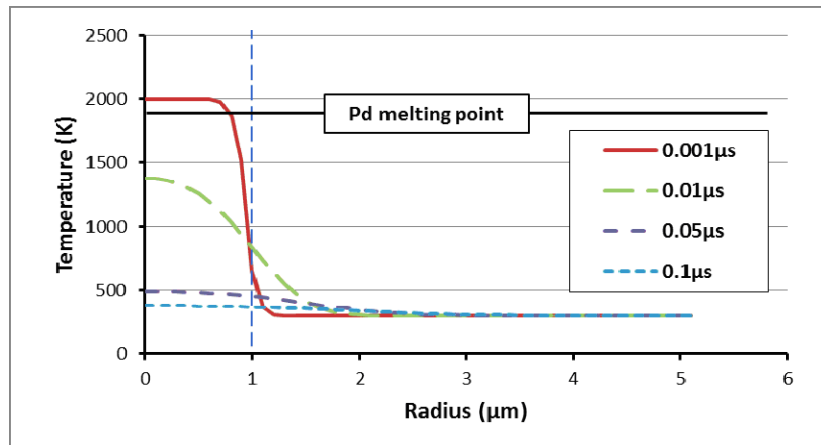


Figure 9. Evolution of the temperature for a 2 μm diameter core – Assumed reaction time is 0.001 μs .

The temperature reaches a maximum at the end of the reaction time τ .

If τ is small, as shown in Fig. 9 for $\tau = 1$ ns and Fig. 11 for $\tau = 100$ ns, the heat loss towards the surrounding metal is still very limited at the end of the reaction. Most of the energy is still confined within the core and the temperature reaches 2000 K in both cases, as can be deduced from Eq. (1) and Fig. 6.

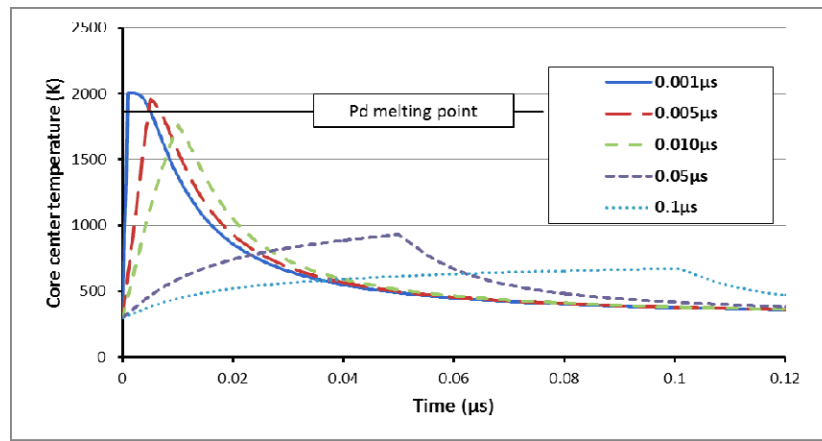


Figure 10. Evolution of the temperature at the centre of a $2 \mu\text{m}$ core – Influence of the reaction time.

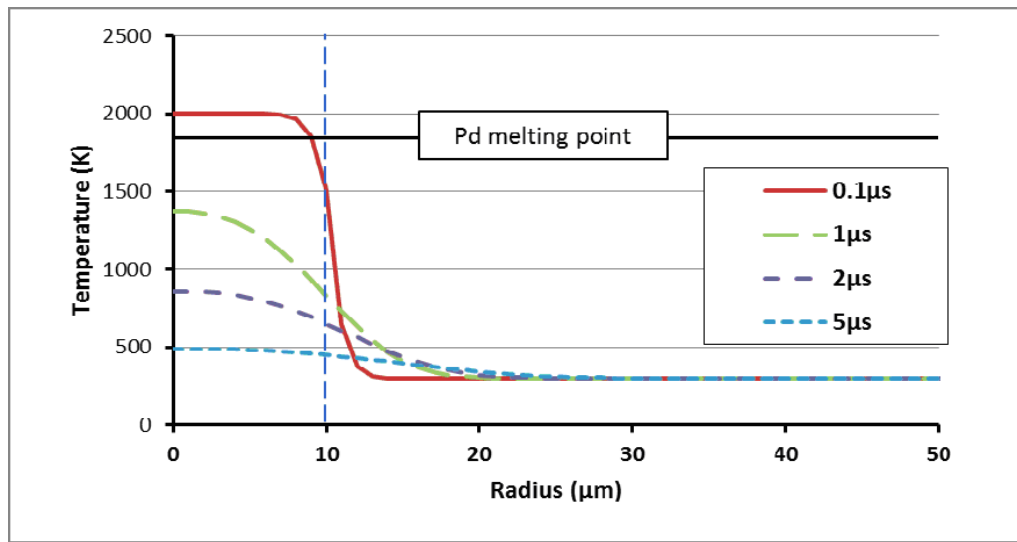


Figure 11. Evolution of the temperature for a $20 \mu\text{m}$ diameter core – Assumed reaction time is $0.1 \mu\text{s}$.

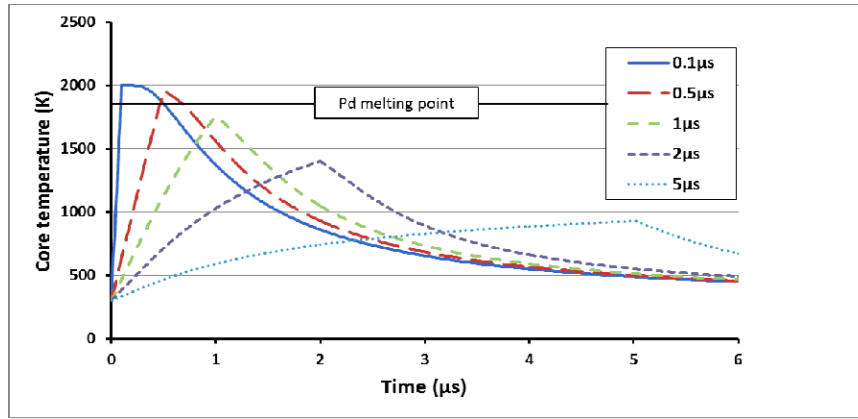


Figure 12. Evolution of the temperature at the centre of a 20 μm core – Influence of the reaction time.

The subsequent cooling by conduction is, however, very rapid. If we define $t_{1/2}$ the time necessary to reduce by half the temperature rise of the core centre, Figs. 10 and 12 show that $t_{1/2}$ is 0.013 μs for the 2 μm core and 1.3 μs for the 20 μm core. We can generalize :

$$t_{1/2} = 3250 d^2, \quad (3)$$

where d is the hot core diameter.

If we use longer reaction times τ , the maximum temperatures reached at the end of the reaction are markedly lower. Conduction takes away the heat as it evolves. Nagel's correlation does not depend on the time. This can be easily explained by this model if we accept that the reaction time τ is probably very short.

τ is probably less than 6×10^{-9} s for the 2 μm crater and less than 6×10^{-7} s for the 20 μm crater. From that, we can even derive a criteria giving the maximum value of τ as follows :

$$\tau < 1500 D^2, \quad (4)$$

where τ is the maximum value of the reaction time (s), and D the crater diameter (m).

This relation does not mean that the reaction kinetics depends on the crater dimension. It only indicates what the longest duration can be. It may be faster, with no relation to the size. However, this equation shows that very small craters can only be created by very fast reactions.

4.2.2. Hot spot cooling by radiation

When the reaction takes place close to the surface, a crater is formed. The surface exhibits a hot spot at this location and the crater ejects some material.

Let us first consider the energy loss into the environment. Because of the high temperature, the hot spot radiates strongly, so that it is necessary to evaluate how much energy the hot core loses by radiation. To do this we assume that:

- The hot spot is a flat circular disk with the same diameter as the crater (an overestimate).

- The temperature is 2000 K.
- The duration is $t_{1/2}$ as per Eq. (3).
- The hot spot radiates like a black body.

The Stefan–Boltzmann equation gives the quantity of energy E_r lost by radiation:

$$E_r = \frac{\pi}{4} D^2 \sigma T^4 t_{1/2}, \quad (5)$$

where D is the crater diameter, σ the Stefan–Boltzmann constant ($5.67 \times 10^{-8} \text{ W m}^{-2} \text{ K}^{-4}$).

We find $E_r = 3.7 \times 10^{-14} \text{ J}$ for the $2 \mu\text{m}$ crater and $E_r = 3.7 \times 10^{-10} \text{ J}$ for the $20 \mu\text{m}$ crater. These values are orders of magnitude lower than E_i . We can therefore conclude that radiation cooling is not a relevant factor in this problem.

4.3. Crater eruption

We now have to examine the crater eruption itself. If the material originally located inside the crater is ejected, this is because mechanical forces are acting on it. It can be assumed that the driving force results from the evolution of gases within the crater. The sources of gas may be:

- Metal vapour resulting from the high temperature.
- Hydrogen (deuterium) present in the palladium hydride.
- Nuclear reaction products.

In the above, it is considered that the temperature reached at the beginning of the crater eruption is about 2000 K. This is much below the palladium boiling point (3236 K). Therefore, the palladium vapour pressure is probably low during the eruption itself.

The quantity of nuclear ashes is probably negligible and can be disregarded.

When LENR reactions are observed, the palladium is heavily loaded with deuterium. At high temperature, the hydride is dissociated [9]. The solubility of deuterium is known to decrease as the temperature increases. In our case, during the eruption, the palladium is molten. The gas pressure build-up is difficult to quantify, because the reaction is very rapid. It is unclear how fast the atoms of deuterium present in the liquid phase combine into D_2 molecules, how gas bubbles can germinate, etc.

Facing these difficulties, we are again obliged to use a very simple model in an attempt to find out the main orders of magnitude of the eruption mechanism.

Should the quantity of hydrogen (deuterium) contained in the hydride instantaneously evolve as gas, the local pressure could be estimated as follows:

- Mass of hydride : $10^4 \text{ kg m}^{-3} = 8.85 \times 10^4 \text{ mol PdD}$ per cubic meter.
- If the gas is released as monoatomic hydrogen, considered as a perfect gas, the equivalent pressure of the gas would be $1.98 \times 10^3 \text{ bar}$ at 0°C . Because the temperature is 2000 K, the gas pressure may be as high as $1.45 \times 10^4 \text{ bar}$.

The actual pressure is difficult to assess. We can nevertheless estimate that the pressure is quite high, possibly ranging between 100 and 20,000 bar.

The mechanism of eruption is probably complicated, but as we are only looking after approximations, the following *ad hoc* model is a first approach:

- The gas pressure P is taken as a variable to study its influence.

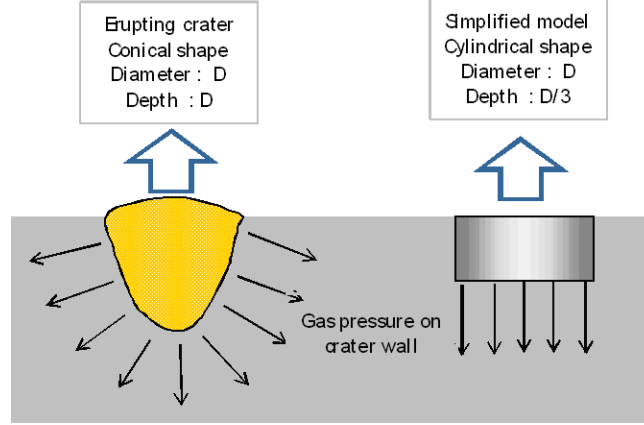


Figure 13. Schematic view of a crater in eruption and simplified modelling. The cylinder in the model has the same volume as the crater.

- The pressure is constant during the eruptive phase and appears instantly.
- The crater having a diameter D is represented by a cylinder perpendicular to the surface, with the same diameter D and a depth $D/3$ to account for the fact that the actual crater has a conical shape, see Fig. 13.
- The gas pressure is exerted on the bottom face of the cylinder and creates a force pushing out the content of the cylinder, as if it were solid.

The eruption duration is defined as the time required to lift the cylinder along a distance equal to its height $D/3$.

We can write the force F exerted at the base of the cylinder:

$$F = \frac{\pi}{4} D^2 P = m \gamma = \frac{\pi}{12} \rho D^3 \gamma, \quad (6)$$

where P is the gas pressure and γ is the acceleration of the cylinder.

The time t_e required to travel the distance $D/3$ during the eruption is:

$$\frac{1}{2} \gamma t_e^2 = \frac{D}{3}. \quad (7)$$

Replacing the value of γ obtained in Eq. (5), we get:

$$t_e^2 = \frac{2}{9} \rho \frac{D^2}{P}. \quad (8)$$

Taking $\rho = 10^4 \text{ kg m}^{-3}$ for the hydride, it gives:

$$t_e = 47.1 D P^{-0.5}. \quad (9)$$

Figure 14 shows the eruption time calculated for different diameters and pressures.

It is instructive to compare the values of t_e with the values of τ given by Eq. (3). Both values are equal when the following equations are satisfied :

$$1500 D^2 = 47.1 D P^{-0.5}, \quad (10)$$

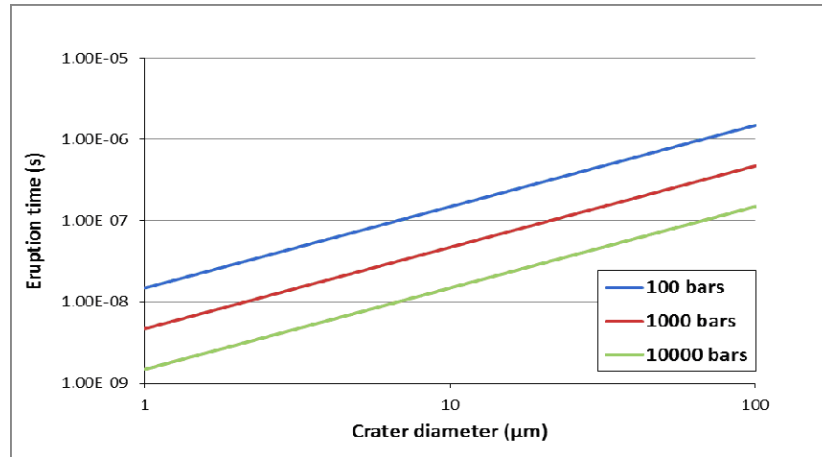


Figure 14. Eruption time calculated for different crater diameters and gas pressures.

$$D = 0.03P^{-0.5}. \quad (11)$$

For example, if the gas pressure is 1000 bar (10^8 Pa), we have $D = 3 \mu\text{m}$.

Craters smaller than this value are cooled down before the eruption is completed. They cannot contain molten material because the metal is quenched by the wall as the eruption proceeds. Larger craters erupt faster than they cool, so that molten material is present in the ejected debris.

5. Discussion of the Results

The correlation established by Nagel gives the energy input for the formation of micro-craters, as seen on the palladium cathodes of LENR experiments.

The simplified modelling approach presented here lacks precision, but gives the orders of magnitude of the time scales of the related phenomena. The event duration ranges from a few nanoseconds to less than a microsecond depending on the crater size.

The cooling of small craters is very fast. It may be so fast that the LENR energy is dissipated by conduction before the temperature reaches the metal melting point. The gas released must however find its way to the outside, tearing off the base metal.

In larger craters, the energy results in the melting of at least a part of the crater content, which is subsequently blown away by the gas, see Fig. 15.

This simple model may explain why the small craters shown in Fig. 4 do not exhibit signs of melting, while the large ones in Figs. 1 and 2 show accumulation of molten metal around the rim.

This model does not give any hint of the LENR mechanism itself. However, the occurrence of such craters, assuming they result from LENR events, invites the following remarks, most of them already pointed out by Nagel [6] :

- LENR reactions are said to be related to some particular behaviour of deuterium atoms incorporated in Pd crystalline structure. The Pd crystals are not rounded, contrary to the large craters. This means that the

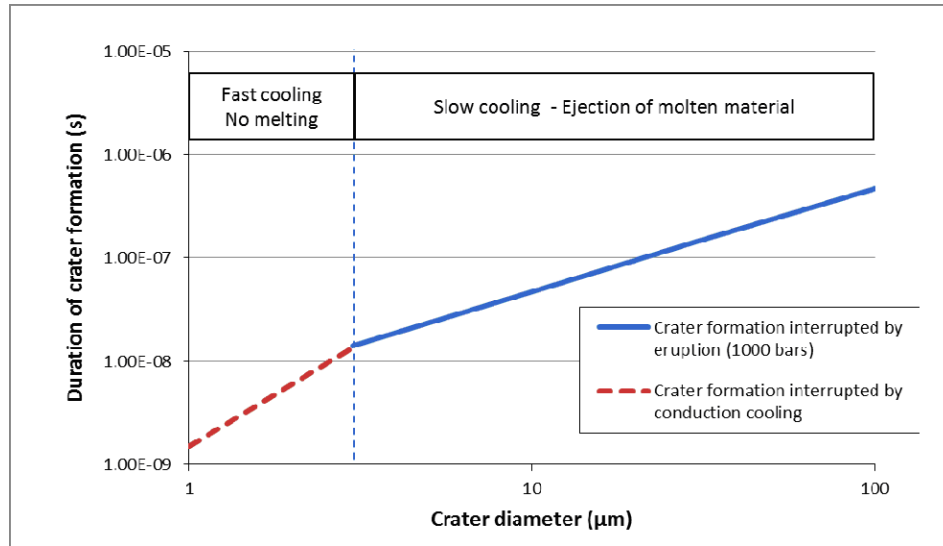


Figure 15. Criteria for the presence of molten material in LENR craters.

dimensions of the LENR sites may be markedly smaller than the final craters.

- Shortly before the reaction starts, the site is obviously at the same temperature as the base metal. The reaction is not initiated because of a high local temperature.
- If all the energy is generated within a site smaller than the crater, the temperature level reached at the end of the nuclear event, before the crater expansion, is considerably higher than the 2000 K value estimated by the crater formation energy correlation (1). Dividing the volume by 10 means a reaction temperature of 20 000 K for example. Maybe, the multiplication factor is much higher.
- If the LENR site is smaller than the crater, the duration of the nuclear reactions is even shorter than the values given for τ in equation (4)
- The crystalline structure supposed to be the matrix of LENR events is completely destroyed by the high temperature. If LENR reactions occur in such sites, they take place in a medium completely out of equilibrium.
- Such high temperatures developed in a very short time mean huge instantaneous powers. If we consider again the Nagel's correlation, the 50 μm conical crater represent an energy of 10^{-4} J. If the LENR site dimension is a 10 μm large cube, the energy density is 10^{11} J m^{-3} , released in less than 150 ns. The instantaneous power is then larger than 6×10^{17} W m^{-3} . These are really microscopic explosions.
- It is tempting to relate such phenomena to some explosions which have been reported by several researchers [10]. It is however not easy to explain how small size explosions can trigger an explosion in a large volume.
- The LENR energy is probably transferred to the surrounding metal via a shock wave, resulting in the formation of the crater, very much like during an underground explosion.
- A possible sequence of the formation of a crater is proposed in Fig. 16:
 - LENR reactions starts on a given site, initially cold, for some reasons which remain to be explained,
 - The reactions develop very fast within the site and the temperature reaches a very high temperature, maybe in the order of several thousands of Kelvins,

- A shock wave transfers the energy to the surrounding metal. The temperature decreases gradually. When the event takes place close to the surface, the shock wave reaches the surface. The temperature is close to 2000 K, at least for the large craters,
 - The gases contained in the hot metal create a pressure build-up, which leads to the ejection of the crater content.
- The explosions are probably accompanied by flashes of visible light. In fact, hot spots have already been observed in the infrared domain [3,11]. The direct observation of the cathodes during the experimentation with a monitoring of the images should make it possible to confirm the mechanisms proposed here.
 - Many craters have a depth of several μm . If we accept that the LENR reactions at the origin of the crater are located near the bottom, this means that the reactions arise far below the surface, measured according to the atom scale.
 - It is even possible that reactions are present at greater depths, not revealed by craters on the outer surface. Szpak et al. detected events underneath the surface during their co-deposition experiments [3]. It would be interesting to check if special metallic features possibly related to deep LENR sites can be observed within the palladium cathodes, which gave excess heat, several tens to hundreds of μm below the surface. This can be done with metallographic techniques on transverse cuts of the cathodes.
 - Such investigations should help to understand better the mechanism of formation of the craters themselves, and to confirm or infirm the hypotheses made here.
 - It is beyond the objective of this paper and the competencies of the author to draw any conclusion regarding the nature of LENR phenomena, but the above raises many points which should deserve further thoughts.

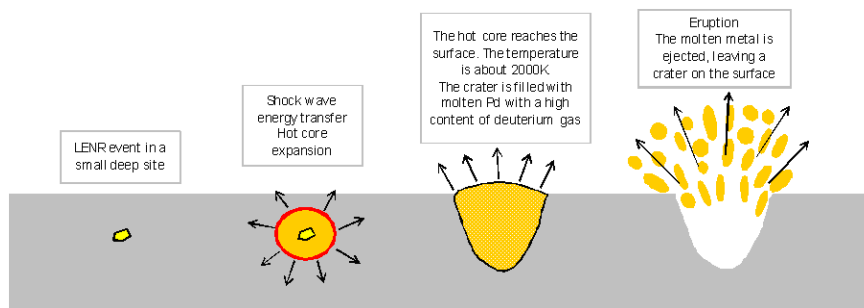


Figure 16. Schematic representation of the formation of a crater.

6. Conclusions

Simple models of heat flow and eruption kinetics give some orders of magnitude of the time scales involved during the formation of the micro-craters observed on palladium cathodes after LENR experiments. The reactions durations are measured in nanoseconds. The model explains the presence or not of molten material around the craters according to their size. The values of time and dimensions mentioned here lead to the conclusion that LENR seem to evolve like microscopic nuclear explosions, at least as far as deuterium loaded palladium cathodes are concerned.

The reactions start in a cold material, so the reactions are not initiated because of a high temperature. Another unexplained phenomenon is responsible for the onset. However, the temperature increases very quickly in an explosive fashion. It is not clear if the reactions continue within the site because of the high temperature, but at the beginning of the shock wave expansion phase, the temperature is so high that any ordered arrangement of atoms can no longer exist.

Further investigations are suggested in order to clarify several aspects:

- Is there a clear relationship between excess heat, LENR phenomena and the presence of craters (as supposed here) , or is excess heat obtained without observation of craters?
- The explosions responsible for the craters must be accompanied by flashes of visible light which may be detected using appropriate experimental setups.
- Metallographic studies on cuts made perpendicular to the cathode surface could show remnants of LENR sites near the bottom of craters. This would give the possible dimension of the LENR sites at the origin of the crater, and hence the maximum temperature reached
- Similar investigations could reveal reactions which occurred deep below the surface without cratering. Their presence would reinforce some theories, and their absence others.

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