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CRÁTERES POR IMPACTO DOBLE

Portada: Image of a double intruder penetrating a granular bed.

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LA FÍSICA DE LAS CAÍDAS DEL SEN

THE PHYSICS OF SEN'S POWER OUTAGES

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En los años 1980's la TV cubana pasaba una cantidad muy limitada de películas de entretenimiento "occidentales". La noche de los sábados era uno de esos raros momentos en que pasaban dos películas "buenas", seguidas por una enorme cantidad de tele-espectadores. Un conocido de uno de los autores (E.A.) que trabajaba en la Despacho Nacional de Carga, relata que los responsables del turno del sábado en la noche debían mirar atentamente esas películas en un monitor de TV dedicado a ello. Apenas terminaba la segunda película, pasaban frenéticamente a ajustar la generación eléctrica despachable del país, para se adaptara a la dramática caída de consumo eléctrico asociada a apagar cientos de miles de televisores al unísono. Este ejemplo ilustra bien uno de los principios básicos para garantizar la estabilidad de una red eléctrica: la necesidad del equilibrio instantáneo entre generación y consumo.

El Sistema Electroenergético Nacional (SEN) fue diseñado para funcionar con grandes turbinas girando (termoeléctricas de petróleo o diésel). Esas turbinas tienen inercia: ejes de enorme masa girando a 60 Hz. Si de repente falla una planta, la inercia sostiene la frecuencia por unos segundos –que pueden resultar críticos para la que no se pierda la estabilidad de la red eléctrica del país.

Un panel solar fotovoltaico representa el otro extremo, pues posee cero-inercia: cuando, por ejemplo, una nube proyecta una sombra, su producción cae a cero en fracciones de segundo. Y ahí se tiene otro tipo de problema: si en ese momento hay muchos paneles en la red y pocas turbinas girando en las termoeléctricas, la frecuencia se desploma. Y, si la frecuencia baja demasiado, el sistema se desconecta sólo, para protegerse. Ocurre entonces la temida "caída del SEN". Este escenario puede involucrar no sólo a los paneles solares, sino a otras fuentes renovables de energía. Un método para agregar "inercia" a estas fuentes es el uso de bancos de baterías que acumulen parte de la energía generada, y la pueden distribuir en el momento que sea necesario para ajustar el delicado balance entre generación y consumo. Lamentablemente, las baterías son relativamente caras.

En pocas palabras: en ausencia de baterías u otros sistemas de almacenamiento de la energía producida, la contribución a la generación eléctrica fotovoltaica no debe ser superior a cierta fracción de la generación total. Así, si salen súbitamente del sistema demasiadas termoeléctricas en un país y la contribución de la generación de energías renovables crece excesivamente, el sistema es mucho más susceptible a sufrir una inestabilidad.

La causa de ésta también puede comenzar por un accidente en la red misma de transmisión de energía.

Esto no es un problema exclusivamente cubano. Por ejemplo, en septiembre de 2016, Australia del Sur vivió un apagón relativamente similar. A las 4:16 de la tarde, una tormenta derribó varias torres de transmisión. En solo dos minutos, la red sufrió seis caídas de tensión consecutivas. Los parques eólicos (que, como los paneles solares, usan inversores electrónicos y no tienen inercia) estaban programados con una protección: si ocurrían demasiadas perturbaciones en poco tiempo, se desconectaban automáticamente. Eso fue exactamente lo que pasó. En menos de siete segundos, 456 megawatts de generación eólica desaparecieron de la red. La interconexión con el sistema vecino se sobrecargó y también se desconectó. Australia del Sur quedó en modo *isla*: sólo con su propia generación, que era insuficiente para la demanda. A las 4:18 de la tarde, más de 850 mil clientes quedaron sin electricidad. [1]. Cuba basa el grueso de su producción eléctrica en termoeléctricas muy viejas (varias de los años 80 del pasado siglo), que sufren una escasez crónica de combustible. Por ejemplo, la termoeléctrica "Antonio Guiteras", con sus cerca de 300 megawatts de potencia nominal [2] y su achacosa caldera –que obviamente requería de una inversión capital desde hace años– es la mayor de la isla.

Impulsada por nuestra crisis energética crónica, y para disminuir la dependencia de combustibles fósiles importados, la isla ha aumentado la participación de la energía solar en su matriz eléctrica del 5.8% a más del 20% en solo un año [3]. Para marzo de 2026, ya operaban 49 parques solares con una capacidad de hasta 1000 MW. Se trata de una expansión masiva con inversión cubana que, según plan, debe llegar a los 2000 MW en un par de años. A ello se suman algunas donaciones provenientes fundamentalmente de China y Vietnam. A pesar de estos avances, el suministro sigue siendo frágil: el déficit de generación térmica provoca apagones muchas horas diarias. Se ha confirmado que el potencial técnico para el desarrollo futuro es enorme, estimando que los techos cubanos podrían generar 2,175 GWh anuales [4]. Adicionalmente, en el país está en proceso de puesta en marcha un primer banco de baterías de 50 MW, que ha de estar instalado cuando éstas líneas salgan a la luz, mejorando en alguna medida la disponibilidad de energía eléctrica a lo largo del día y la estabilidad de la red como un todo. Vale subrayar que esta transición de la matriz energética está siendo asesorada muy de cerca por

el Laboratorio de Fotovoltaica del Instituto de Ciencia y Tecnología de Materiales (IMRE) de la Universidad de La Habana, que fue reconocido por la Alianza Solar Internacional como el primer y único Centro STAR en América Latina una distinción que avala su capacidad para promover estándares internacionales en tecnología solar [5]. Como hemos sugerido más arriba, un problema muy serio asociado a esta acelerada y necesaria transformación de la matriz energética es no-trivial: asimilar tanta generación sin inercia. Y no sólo por la existencia de termoeléctricas muy viejas con paradas frecuentes, sino por la carencia crónica de combustible que no permite que los grupos electrógenos sean manipulados para “adaptarse dinámicamente” a las fluctuaciones. El resultado lo hemos vivido repetidamente: apagones por inestabilidad dinámica. Aunque obviamente la buena organización (o falta de ella), sentido de la previsión (o falta de él), los factores externos (como el cerco petrolero impuesto desde inicio de este año) y la acelerada presencia de fuentes energéticas renovables son elementos fundamentales que deciden las “caídas del SEN”, la Física y las ciencias de la computación poseen sin duda un nicho científico para contribuir a su estabilidad, más allá de diseño mismo de los paneles y la electrónica asociada. Un artículo de revisión de Witthaut y colaboradores [6] ilustra el enorme campo que se abre ante la física estadística en términos de la modelación de los fenómenos colectivos y no-lineales asociados a las redes eléctricas sometidas a fluctuaciones, que podrían permitir el rediseño y/o control de dichas redes sobre la base de datos reales.

La Física cubana ya ha salido en ayuda del SEN. Comenzando por los dispositivos en sí mismos, podemos decir que el conocimiento acumulado en el Laboratorio de Fotovoltaica de la Universidad de la Habana sobre las tecnologías de fabricación de celdas solares (en especial de silicio) [7], ha permitido asesorar sobre los módulos fotovoltaicos que podrían adaptarse mejor a las condiciones cubanas de alta radiación, alta temperatura ambiental y altos valores de humedad relativa.

Por su parte, los colegas del Instituto de Meteorología (Insmet) han desarrollado un modelo de pronóstico de generación solar a partir de variables climáticas que se utiliza desde hace años para la gestión de la estabilidad del SEN [8], el cual está siendo perfeccionado con la ayuda de herramientas de Inteligencia Artificial. Dentro de este tema, se ha estudiado en otros lares la influencia de la forma de las nubes en la forma de sus sombras, con evidente impacto en la generación solar [9]. Curiosamente, para ello se ha utilizado la dimensión fractal de las nubes para cuantificar su forma, un tema en el que colegas de la Facultad

de Física de la Universidad de La Habana, el Instec y el Insmet han colaborado en el pasado [10].

Otra contribución de la Física y la matemática aplicada a la estabilidad del SEN podría ser el estudio de las series temporales de la frecuencia de la red medida en una serie de puntos, y crear un algoritmo para predecir posibles desviaciones “caóticas” de la frecuencia deseada, en tiempo real. Semejante medición no parece especialmente difícil, si se usan sensores distribuidos.

Desde luego, esto nos recuerda a una serpiente que se muerde la cola: para que exista la estabilidad de cómputo (¡y humana!) necesaria para que nuestros físicos “se metan” en estos asuntos, no sólo hace falta la colaboración de las instituciones: hace falta que haya estabilidad en el fluido eléctrico.

REFERENCIAS

- [1] Australian Energy Market Operator (AEMO), “Black System South Australia 28 September 2016 - Final Report”, 2017.
- [2] “Power Plant Profile: Antonio Guiteras Plant, Cuba”, Power Technology, <https://www.power-technology.com/data-insights/power-plant-profile-antonio-guiteras-plant-cuba/>.
- [3] M. S. Calvo y H. S. Lee, Energy Reports **14**, 254 (2025).
- [4] “As the US starves it of oil, Cuba is pulling off one of the fastest solar revolutions on the planet with China’s help”, CP24, <https://www.cp24.com/news/world/2026/05/13/as-the-us-starves-it-of-oil-cuba-is-pulling-off-one-of-the-fastest-solar-revolutions-on-the-planet-with-chinas-help/> (2026).
- [5] “Fotovoltaica UH Star”, Universidad de La Habana, <https://www.uh.cu/2025/08/08/fotovoltaica-uh-star/> (2025).
- [6] D. Witthaut, F. Hellmann, J. Kurths, S. Kettemann, H. Meyer-Ortmanns y M. Timme, Rev. Mod. Phys. **94**, 015005 (2022).
- [7] L. Vaillant-Roca, Rev. Cubana Fis. **40**, 2 (2023).
- [8] I. Borrajo-Montejo, A. Roque-Rodríguez, J. C. Peláez-Chávez, M. Hinojosa, K. Naranjo-Villalón y M. Sierra-Lorenzo, Ingeniería Energética **44**, 66 (2023).
- [9] G. M. Lohmann, A. Hammer, A. H. Monahan, T. Schmidt y D. Heinemann, Solar Energy **150**, 255 (2017).
- [10] A. R. Batista-Tomás, O. Díaz, A. J. Batista-Leyva y E. Altshuler, Quart. J. Roy. Meteorol. Soc. **142**, 938 (2016).

BELIEF PROPAGATION WITH INFORMED INITIALIZATION IN COMBINATORIAL OPTIMIZATION PROBLEMS

PROPAGACIÓN DE MENSAJES CON INICIALIZACIÓN INFORMADA EN PROBLEMAS DE OPTIMIZACIÓN COMBINATORIA

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In this work, we study the behavior of the Belief Propagation (BP) algorithm in solving two combinatorial optimization problems: 3-SAT and 3-XORSAT. We examine the performance of BP on planted instances, applying the algorithm with a fraction of the variables fixed from the beginning. The probability of reaching any solution using this informed initialization displays abrupt changes with the number of fixed variables. In both problems, BP requires fixing a smaller fraction of variables than the Monte Carlo algorithm to solve a given instance. We also extended a known analytical description of the Unit Clause Propagation Algorithm to accurately predict BP's behavior with an informed initialization for 3-XORSAT in random regular graphs.

En este trabajo estudiamos el comportamiento del algoritmo Belief Propagation (BP) en la resolución de dos problemas de optimización combinatoria: 3-SAT y 3-XORSAT. Aplicamos BP a la versión plantada de estos problemas cuando una fracción de las variables está fija desde el inicio. La probabilidad de resolver una instancia usando esta inicialización informada muestra cambios abruptos con el número de variables fijadas. En ambos problemas estudiados BP requiere menos variables fijadas que el algoritmo de Monte Carlo para converger a una solución. Finalmente, extendemos una conocida descripción analítica del algoritmo Unit Clause Propagation para predecir con precisión el comportamiento de BP aplicado al 3-XORSAT en grafos aleatorios regulares con inicialización informada.

Keywords: combinatorial optimization (optimización combinatoria), planted model (modelo plantado), belief propagation (propagación de creencias)

I. INTRODUCTION

Most optimization problems are formulated via the extremization of some function $f(\vec{x})$, of N variables ($\{x\}$) that must satisfy specific constraints. For continuous variables, if the function to extremize and the constraints are linear, the exact solution of the problem is obtained using Linear Programming, a well-known general algorithm [1]. On the other hand, when the function is non-linear and the variables are discrete, we step into a field where problems are usually more difficult [2]. In computer science, these problems are usually recognized as *combinatorial optimization problems* and have common grounds with the field of disordered systems in statistical physics [3].

This connection between combinatorial optimization and statistical physics has triggered the efforts to understand the structure of the solution space of some problems [4, 5] and the (sometimes surprising) capacity of algorithms to find solutions [6–8]. However, despite the advances in the field, we lack a general algorithm to efficiently solve every problem of this type and must approach them with tailored heuristics [9–11].

Therefore, understanding the performance of general and (in many cases) successful algorithms for combinatorial optimization problems, such as Simulated Annealing [12, 13]

and Belief Propagation (BP) [14, 15], continues to be a very active research area.

Here, we move forward in this direction by studying BP's performance solving K-SAT and K-XORSAT problems when it is provided with an informed initialization. Both K-SAT and random K-XORSAT are very well-known combinatorial optimization problems and have been widely used as benchmarks to test algorithmic performance [16–20]. In our informed initialization, a fraction of the variables is fixed from the beginning and then BP is run to find the right assignment of the rest of the variables of the system. Moreover, we extend some of the results in Ref. [14] to understand the behavior that we observe when BP is applied to K-XORSAT instances on random regular graphs.

The rest of the work is organized as follows. In the next section, we present in detail the two problems, including some known results to contextualize our work. The algorithm, BP, is introduced in the following section titled *Belief Propagation*. Then, we compare the performances of BP and Monte Carlo (MC) when we use informed initializations. Finally, we present the conclusions of our work.

II. TWO PROBLEMS

The K-SAT problem deals with clauses formed by the logical OR of K variables. Its computational hardness depends on the density of clauses $\alpha = \frac{M}{N}$, where M is the number of clauses and N is the number of variables. The problem is typically defined on random factor graphs with Poisson (Erdős–Rényi) connectivity. As α increases, the solution space undergoes a sequence of sharp phase transitions. For small α the system is always solvable. At any given K , there is a threshold α_s such that, for $\alpha > \alpha_s$ there are no satisfying assignments with high probability when the size N of the formula is large. On the other hand, for $\alpha < \alpha_s$ a formula will have a satisfying assignment with high probability when the size N of the formula is large. For $K=3$, for example, we have $\alpha_s \approx 4.267$ [4, 21]. This sharp change around α_s is called the SAT-UNSAT transition.

Notably, there is another transition at some $\alpha_d < \alpha_s$ [4, 22] where the system enters a dynamical glassy phase, characterized by clustering of solutions and slow relaxation dynamics, often referred to as the dynamical transition. For $K=3$, we have $\alpha_d \approx 3.86$. It is often considered that hard-to-solve instances appear in the region $\alpha_d < \alpha < \alpha_s$, identifying the location of α_d as the onset of algorithmic hardness. However, the actual relevance of this threshold for real algorithms is not completely clear, since one can find several heuristics capable of reaching solutions well beyond α_d [6, 15, 23–26].

On the other hand, the K-XORSAT problem involves logical clauses that are satisfied when the sum modulo 2 (i.e., XOR) of K Boolean variables equals a fixed value. When this problem is translated into statistical physics via a mapping to spin variables—replacing Boolean values $\{0, 1\}$ with Ising spins $\{\pm 1\}$, it becomes equivalent to the ferromagnetic p -spin model ($p = K$), a paradigmatic system in spin-glass theory [16, 17]. In this formulation, each clause corresponds to a K -body interaction that favors the alignment of the spins, leading to a ferromagnetic Hamiltonian. This connection has made K-XORSAT a valuable benchmark for studying algorithmic thresholds and phase transitions in disordered systems [16–18].

The SAT-UNSAT and dynamic transitions also occur in random K-XORSAT at some α_d and α_s , respectively. However, there is a key difference with K-SAT: solutions of K-XORSAT can be found in polynomial time for any α up to α_s , using Gaussian elimination. In other words, we already know an efficient algorithm that solves the problem whenever this is possible. This does not mean that K-XORSAT is an easy problem. It is widely accepted that, when one restricts oneself to local algorithms such as BP or MC, the onset of hardness occurs exactly at α_d . For large K , it has been rigorously proven that finding a solution of K-XORSAT is indeed hard in the region $\alpha_d < \alpha < \alpha_s$ if one uses a local algorithm [27, 28].

In the physics literature, these two problems are usually defined using N binary variables $s_i = \pm 1$, with $i = 1, \dots, N$. Inspired by condensed matter physics, these variables are usually called spins. The combinatorial optimization task

is to find a configuration $\vec{s}^*$ that minimizes the following Hamiltonians:

1. K-XORSAT:

$$H(\vec{s}) = - \sum_{a=1}^M J_a \prod_{i \in a} s_i \quad (1)$$

where $J_a = 1$ in the original formulation of the problem, corresponding to the ferromagnetic p -spin model. Here, we will also allow $J_a = \pm 1$ with equal probability, which in turn corresponds to the disordered p -spin. To simplify the setting, for K-XORSAT we construct $H(\vec{s})$ such that each variable i belongs to the same number of clauses, denoted by c . This builds a c -regular K -uniform random hypergraph.

2. K-SAT:

$$H(\vec{s}) = \sum_{a=1}^M \prod_{i \in a} \frac{1 - J_i^a s_i}{2} \quad (2)$$

where J_i^a indicates whether variable s_i is affirmed ($J_i^a = 1$) or negated ($J_i^a = -1$) in clause a . As usual, here we choose the clauses in the formula uniformly at random among all possible clauses. Then, each variable i belongs to a number of clauses that is Poisson distributed with mean αK .

In the physics nomenclature, the optimal configuration $\vec{s}^*$ is the ground state of the corresponding Hamiltonian at temperature $T = 0$.

To study the performance of algorithms, it is convenient to use *planted instances*, where the existence of at least one solution is guaranteed [29, 30]. The procedure used to build the so-called planted solution depends on the problem of interest, but the general idea is usually the same. One starts by pre-assigning values to N variables (initially disconnected), and then defines a graph of interactions such that the pre-assigned configuration is a solution to the problem.

In our case, these instances are constructed as follows:

1. **random K-XORSAT:** Choose N variables $s_i = \pm 1 \forall i$ with probability $1/2$ to form a configuration $\vec{s}^*$. Then group these variables into M clauses (with indexes $a = 1, \dots, M$) that are also selected uniformly at random. Regardless of the outcome, $\vec{s}^*$ will be the solution of an instance where the J_a are defined as $J_a = \prod_{i \in a} s_i \forall a$. The Hamiltonian (1) takes its minimum value ($H(\vec{s}^*) = -M$) when we build $\vec{s}^*$ and all the J_a following these rules [30].
2. **random K-SAT:** Choose N variables $s_i = 1 \forall i$ to form $\vec{s}^*$. Then group these variables into M clauses (with indexes $a = 1, \dots, M$) that are also selected uniformly at random. All the clauses, of course, contain K variables and one needs to define the corresponding K parameters J_i^a . For every clause a , exclude only the case where $\forall i \in a$, and randomly extract one among all other possible choices for J_i^a , $J_i^a = -1$ and randomly extract one among all other possible choices for J_i^a . This automatically constructs a

Hamiltonian (Eq. (2)) such that $H(\vec{s}^*) = 0$, thus $\vec{s}^*$ is a solution. In practice, we set the clauses with k negated variables to appear with probability p_k , $p_0 = 1/4$, $p_1 = 0$, and $p_2 = 1/4$ and $p_3 = 0$ following reference [29].

This work addresses a key question on algorithmic performance in planted instances: *What is the minimum fraction of variables that must be fixed to find a solution using Belief Propagation?*. This is answered in two contexts: i) when the variables are fixed randomly, and ii) when the variables are fixed to their correct values. In each scenario, we compare the behavior of the BP algorithm with the results of the MC algorithm.

III. BELIEF PROPAGATION

Combinatorial optimization problems involve minimizing a certain cost function, called *Hamiltonian* or energy in physics. Written generically, this function is:

$$H(\vec{s}) = \sum_{a=1}^M \Psi_a(s_i, i \in a) - \sum_{i=1}^N h_i s_i \quad (3)$$

where the term Ψ_a is a function of the spins contained in the clause with index a . Essentially, all Ψ_a functions must be minimized simultaneously. Another important definition is the average magnetization:

$$m(\vec{s}) = \frac{1}{N} \sum_{i=1}^N s_i. \quad (4)$$

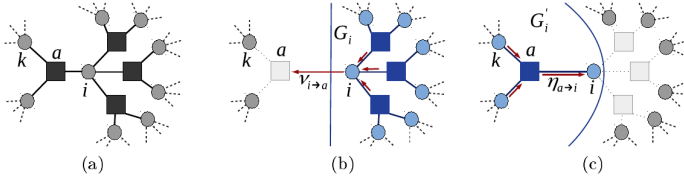


Figure 1. Visualization of the BP algorithm in the factor graph section of panel (a). In panel (b), the connection between i and the clause a is removed. The message $v_{i \to a}(s_i)$ from i to a is the local probability distribution associated with the spin s_i in the remaining subgraph G_i (colored in blue). In panel c), almost all the connections involving s_i have been removed, leaving only its connection with a . The message $\eta_{a \to i}(s_i)$ from a to i is the local probability distribution of s_i in the subgraph G'_i (colored in blue).

The magnetization $m(\vec{s})$ tells us about the collective orientation of the spins, which can also be guided by the local external fields h_i in Eq. (3).

The cavity method provides a way to determine local probability distributions in tree-like graphs [3,4,31]. The main idea is to make small modifications of the graph to define new *cavity* marginals or messages $v_{i \to a}(s_i)$ and $\eta_{a \to i}(s_i)$ (see Fig. 1). These are used afterwards to get back the marginals in the original graph $p(s_i)$.

One key point of the scheme is the BP self-consistency equations, which must be updated iteratively to obtain the fixed-point messages:

$$v_{i \to a}(s_i) = \frac{e^{\beta h_i s_i}}{Z_{i \to a}} \prod_{b \in \delta i \setminus a} \eta_{b \to i}(s_i) \quad (5)$$

$$\eta_{a \to i}(s_i) = \frac{1}{Z_{a \to i}} \sum_{s_{a \setminus i}} e^{-\beta \Psi_a(s_i, j \in a)} \prod_{k \in a \setminus i} v_{k \to a}(s_k) \quad (6)$$

where $\beta = 1/T$ is the inverse temperature and $Z_{i \to a}$ and $Z_{a \to i}$ are normalization constants. The symbol $b \in \delta i \setminus a$ represents the set of all clauses that contain i , except a . On the other hand, $a \setminus i$ is the set of variables that belong to clause a , except for i . Therefore, the sum $\sum_{s_{a \setminus i}}$ goes over all the configurations of the spins associated with the spins in $a \setminus i$.

The BP equations provide an exact solution for problems defined on locally tree-like graphs, meaning the probability of encountering closed cycles is null or very low. Note that if $h_i \rightarrow \pm\infty$, the variable-to-factor node messages in Eq. (5) become $v_{i \to a}(s_i) = \Theta(h_i s_i)$, where $\Theta(x)$ is the Heaviside function. In other words, the spin is fixed towards the orientation of the local field. Once the cavity marginals $v_{i \to a}(s_i)$ and $\eta_{a \to i}(s_i)$ are obtained, the local probabilities can be determined as:

$$p(s_i) = \frac{e^{\beta h_i s_i}}{Z_i} \prod_{a \in \delta i} \eta_{a \to i}(s_i) \quad (7)$$

$$p(s_i, i \in a) = \frac{1}{Z_a} e^{-\beta \Psi_a(s_i, i \in a)} \prod_{i \in a} v_{i \to a}(s_i) \quad (8)$$

where Z_i and Z_a are normalization constants and $\Psi_a(s_a)$ is the weight function. Notice that, by construction, at zero temperature BP concentrates on the ground state of the corresponding Hamiltonian (with all the products equal to one). This occurs because in the limit $\beta \rightarrow \infty$, the terms related to the lowest energies dominate the exponential functions in Eq. (8). Thus, if the fixed-point iteration converges, BP gives positive weight only to configurations compatible with the ground state.

IV. RESULTS

This section is divided into two parts. First, we show and discuss the behavior of BP and MC on the random 3-XORSAT problem, and then we move towards the study of the random 3-SAT problem. We remind the reader that we define our graphs of interest using the planted model defined above, in the section "Two Problems". Then, the goal is to test whether BP is able to find the planted or another solution as a function of some initial information about it.

The results are compared with the output of the MC algorithm, also with informed initialization. For the latter, we chose the well-known Metropolis dynamic rule [32]. In each step, this algorithm chooses a variable uniformly at random and

proposes to invert its value. If the change diminishes the number of unsatisfied clauses, *i.e.*, if the energy's variation $\Delta H(s_i \rightarrow -s_i)$ is negative, the change is accepted. If $\Delta H(s_i \rightarrow -s_i) > 0$, the proposal is accepted with a probability that is proportional to $\exp(-\beta \Delta H(s_i \rightarrow -s_i))$.

IV.1. 3-XORSAT

We start our runs by fixing first a fraction (ϕ) of the spins. We consider two possibilities: i) these spins are fixed randomly, and ii) they are fixed as defined by the planted model. Once a fraction of the spins are fixed, we run BP and MC at very low temperatures (looking for the ground state of the system). In all the cases considered here, BP converged.

In Fig. 2 we show the mean absolute local magnetization $|m| = \sum_i |m_i|/N$ as a function of ϕ as obtained from BP, where $m_i = \sum_{s_i} s_i p(s_i)$ is the local magnetization. In the upper panel, a fraction ϕ of the spins is fixed as in the planted model. In the lower panel, a fraction ϕ of the spins is fixed in random positions.

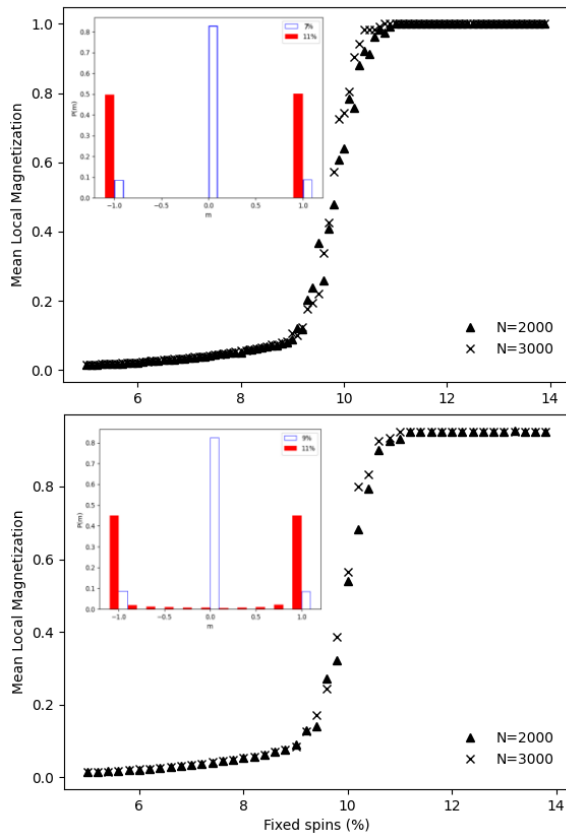


Figure 2. Behavior of the average absolute local magnetization returned by BP as a function of the percentage of fixed spins. Results are obtained for planted 3-XORSAT instances in random regular hypergraphs with connectivity $c = 4$. We imposed strong local fields in random positions and waited for BP's convergence at $T = 0.1$. Each point represents the average of 100 different runs. The inserted graphic displays a frequency histogram of local magnetizations for two distinct percentages of fixed spins. **Top panel:** Variables are fixed towards the planted solution. **Bottom panel:** Variables are fixed to random values.

In both cases, when the fraction of fixed spins $\phi < 10\%$ is low, BP finds paramagnetic solutions, $|m| \sim 0$. The local

magnetizations m_i at most sites i are close to zero (see the histograms of m_i in the insets). Around $\phi \sim 10\%$ the absolute magnetization $|m|$ grows abruptly, and as ϕ increases, the spins magnetize ($|m| \sim 1$). Notice, however, that when the fraction ϕ of the spins is initially fixed in random directions (bottom panel), the algorithm finds a solution in which some of the spins are not fully magnetized. In this case, the solution of BP can not be directly transformed into a ground state configuration.

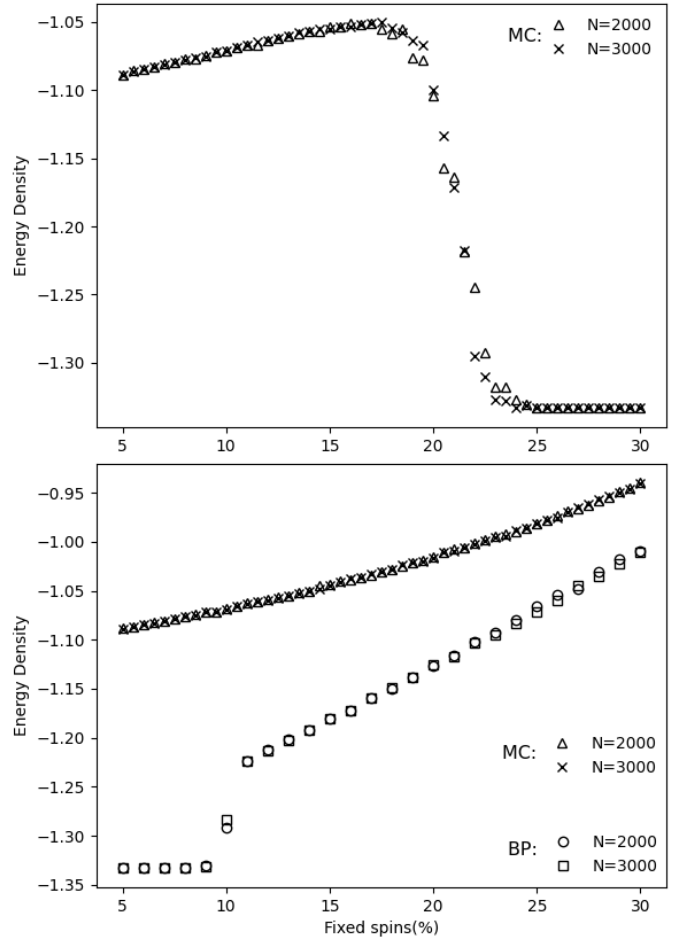


Figure 3. Final energy density returned by MC and BP as a function of the percentage of spins fixed. Results are obtained for the planted 3-XORSAT in random regular hypergraphs with connectivity $c = 4$. We imposed strong local fields in random positions and waited until convergence at $T = 0.1$. Each point represents the average of 100 different runs of the corresponding algorithm. **Top panel:** Spins are fixed towards the planted solution. Points are the result of MC runs. **Bottom panel:** Spins are fixed to random values. The panel shows results for MC and BP.

Indeed, to determine whether the distributions obtained from BP correspond to solutions, it is important to look at their local magnetization. When $m_i = 1$ ($m_i = -1$), one can safely set the corresponding spin to $s_i = 1$ ($s_i = -1$). In the cases where $|m_i| < 1$ for some i , one would have to design a subsequent way to assign s_i . Even when giving local distributions that are not fully magnetized, BP can output a small energy. In the particular case of K-XORSAT, when the local distributions $p(s_i, i \in a)$ give zero weight to the configurations that do not satisfy the clause a , we get the minimum energy. It is not necessary that $p(s_i, i \in a)$ selects one

specific configuration among the satisfying assignments. It is the informed initialization, fixing a subset of variables, which forces BP to converge to a specific solution.

Therefore, it does not make sense to plot the energy obtained from BP when the informed initialization coincides with the planted solution. This energy is always the minimum possible. At this point, we remind the reader that the minimum energy density (energy per variable) for the K-XORSAT is $e_{\min} = -M/N$, which for regular hypergraphs with connectivity $c = 4$ and $K = 3$ coincides with $-c/K = -4/3 \approx -1.333$. However, this is not the case with the MC algorithm, which does not output local probability distributions but actual configurations.

In the top panel of Fig. 3, we show the results of MC when a fraction ϕ of the spins is oriented as in the planted model. When ϕ is small, the informed initialization does not seem to be helping MC. The energy indeed increases slowly when ϕ increases away from zero. Then, around $\phi \approx 18\%$, the informed initialization actually starts helping the algorithm to find the way towards the solution. Notice that the fraction of spins needed to actually recover the minimum energy of the system with MC ($\phi > 22\%$) is larger than the one obtained with BP ($\phi > 10\%$).

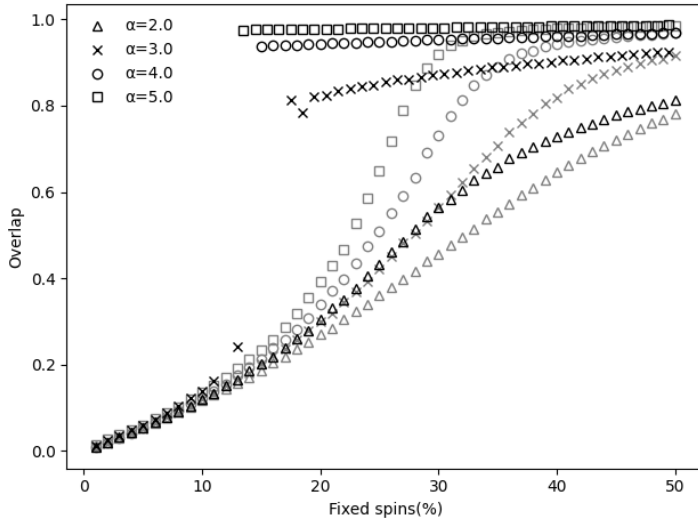


Figure 4. Comparison between the analytical description of UCP, the results of BP and MC runs for 3-XORSAT instances defined over random regular hypergraphs with connectivity $c = 4$. The graphic shows the overlap with the planted solution as a function of the percentage of spins fixed towards a planted solution. We imposed strong local fields in random positions and waited until convergence at $T = 0.1$. Note that BP and UCP reach the planted solution with a smaller fraction of fixed spins than MC. Each point represents the average of 100 different runs.

On the contrary, when the spins are fixed in random positions, it is useful to study the energy obtained after running BP, which can be seen in the bottom panel of Fig. 3. For $\phi < 10\%$, BP gives a small magnetization (see the bottom panel of Fig. 2) and the minimum possible energy $e \approx -1.333$. In this region, the output cannot be directly translated into actual solutions. For $\phi > 10\%$, as soon as the magnetization jumps to large values, the energy departs from the minimum, going up and away from the ground state. Although the fraction of fixed

variables forces BP to converge to specific configurations, these are not solutions. The results indicate that even a small fraction of variables fixed in random positions can effectively obscure the planted solution. However, notice that BP consistently maintains lower energy values than MC in the same scenario. Therefore, from Figs. 2 and 3 we conclude that for $\phi > 10\%$ the output of BP is a set of marginals m_i , almost 90% of which are $m_i = \pm 1$ (see the inserted graphic in the bottom panel of Fig. 2), and which correspond to relatively low energies. These can be easily translated into near-optimal configurations of the problem by taking $s_i = \text{sign}(m_i)$ for all sites.

We also measure the overlap between the solution found by the algorithms ($\vec{s}^{\text{BP}}$, or $\vec{s}^{\text{MC}}$) and the planted solution $\vec{s}^*$. One can define this overlap between any two configurations as a normalized dot product: $Q(\vec{s}, \vec{s}^*) = 1/N \sum_i s_i s_i^*$. In Fig. 4, we compare the overlap between the configurations found with BP and MC and the planted solution as a function of ϕ . The results are consistent with the analysis of the energy shown in Fig. 3. As can be easily seen, BP finds the planted solution already for $\phi > 10\%$, while MC converges to it only when $\phi > 22\%$ of the spins are fixed.

The results in Fig. 4 are analogous to the ones in Fig. 4 of Ref. [33]. However, there are some key differences. First of all, Ref. [33] deals with the ferromagnetic case ($J_a = 1$), while Fig. 4 is for the disordered case (3-XORSAT) with $J_a = \pm 1$. In the former, the magnetization is equivalent to the overlap with the ferromagnetic solution. In the latter, we plant $s_i = \pm 1$ at random and the magnetization is always zero, forcing us to measure the overlap. The second formal difference is that Ref. [33] compares MC with the results of the Cavity Master Equation (CME) [34], while we compare MC with BP. Nevertheless, Ref. [35] later demonstrated that, for dynamics that satisfy detailed balance, the fixed points of the CME are equivalent to BP. Thus, in this case, BP can also be seen as a faster way to compute the fixed points of the CME, improving the procedure used in Ref. [33].

To understand the behavior of BP, we can follow an approach developed in [14]. Let us imagine that what BP is doing is just following a simple rule: whenever $K - 1$ variables in a clause are fixed, the remaining variable is also fixed by BP to the only possible value satisfying the clause. Indeed, remember that in the K-XORSAT the local constraints are satisfied only if the products $\prod_{i \in a} s_i$ are all equal to one. Therefore, knowing the values of the variables s_j , with $j \in a \setminus i$, directly gives only one possibility for the remaining s_i to satisfy the clause a .

The algorithm that proceeds like this, by propagating such logical implications throughout the graph, is called Unit Clause Propagation (UCP) and was already described using differential equations in Ref. [14] for random hypergraphs with Poisson connectivity. Here, we extend those results to the case of random regular hypergraphs. The initial condition for UCP is that a fraction ϕ of variables is already assigned (fixed). At each time step, UCP chooses a clause with $K - 1$ fixed variables, and sets the remaining one to the only possible satisfying value. Therefore, if we measure the time t in Monte Carlo steps, each consisting of N simple UCP iterations, we

get a fraction of fixed variables that grows as $\theta(t) = \phi + t$. Thus, what we need to compute is the limit $\theta_\infty = \lim_{t \rightarrow \infty} \theta(t)$, to get the final fraction of fixed variables.

Let us define $\lambda(t) = 1 - \phi - t$ as the density of variables that are still unassigned at time t , and $\rho_\kappa(t)$ as the density of clauses containing κ unassigned variables at time t . For the latter, we have the differential equation:

$$\frac{d\rho_\kappa(t)}{dt} = -\delta_{\kappa,1} + \frac{(c-1)}{\sum_{\kappa'=0}^K \kappa' \rho_{\kappa'}(t)} \left\{ (\kappa+1) \rho_{\kappa+1}(t) - \kappa \rho_\kappa(t) \right\} \quad (9)$$

At each time step, UCP assigns a value to one variable, converting a clause with $\kappa = 1$ unassigned variables into a clause with $\kappa = 0$ unassigned variables. This explains the term $-\delta_{\kappa,1}$ in the derivative. By doing so, UCP also affects the other $c-1$ clauses that contain the newly assigned variable. At time t , each one of these other *neighboring* clauses will still have κ unassigned variables with probability $\kappa \rho_\kappa(t) / \sum_{\kappa'} \kappa' \rho_{\kappa'}(t)$. Therefore, ρ_κ must increase because some of the "neighboring" clauses with $\kappa+1$ unassigned variables will pass to have κ unassigned variables after each iteration. This explains the term $(c-1)(\kappa+1) \rho_{\kappa+1}(t) / \sum_{\kappa'} \kappa' \rho_{\kappa'}(t)$ in the derivative. In the same way, the term $(c-1) \kappa \rho_\kappa(t) / \sum_{\kappa'} \kappa' \rho_{\kappa'}(t)$ takes into account the neighboring clauses that go from κ to $\kappa-1$ unassigned variables.

Now, we must solve Eq. (9) with the initial condition:

$$\rho_\kappa(0) = \frac{c}{K} \binom{K}{\kappa} (1-\phi)^\kappa \phi^{K-\kappa} \quad (10)$$

To do it, it is enough to follow the same procedure as in Appendix A.1 of Ref. [14], and we obtain:

$$\rho_1(t) = c(1-\phi) [b(t)]^{c-1} \left\{ b(t) - 1 + \left[\theta + (1-\theta)(1 - [b(t)]^{c-1}) \right]^{K-1} \right\} \quad (11)$$

where $b(t) = [(1-\phi-t)/(1-\phi)]^{1/c}$.

Eq. (11) is valid only for the time interval when UCP is still running. As discussed above, the algorithm will stop at the time t^* when it exhausts the clauses with only one unassigned variable, that is, when $\rho_1(t^*) = 0$. To calculate the final fraction of variables assigned by UCP ($\theta(t^*) = \phi + t^*$), given the initial fraction of fixed variables ϕ , and the values of K and c , we need to numerically obtain the time t^* that solves the equation:

$$b(t^*) - 1 + \left[\theta + (1-\theta)(1 - [b(t^*)]^{c-1}) \right]^{K-1} = 0 \quad (12)$$

In Fig. 4 we also show this analytical description (continuous lines). We compare it with the overlap between the marginals

of BP and the planted solution. The agreement is very good, and we believe the differences are due to finite-size effects in the numerical analysis with BP. Using UCP, we estimate with more precision that the abrupt change in overlap occurs at $\phi_c = 0.09575(5)$.

These results indicate that the fundamental mechanism used by BP to find a correct final assignment is analogous to the way UCP works. It propagates logical implications throughout the graph by assigning the variables that belong to clauses with other $K-1$ already assigned variables. Below ϕ_c , it does not go very far and assigns a few variables in total. On the other hand, a small fraction of initially fixed variables $\phi \geq \phi_c$ provokes an avalanche of assignments that ultimately covers the whole graph.

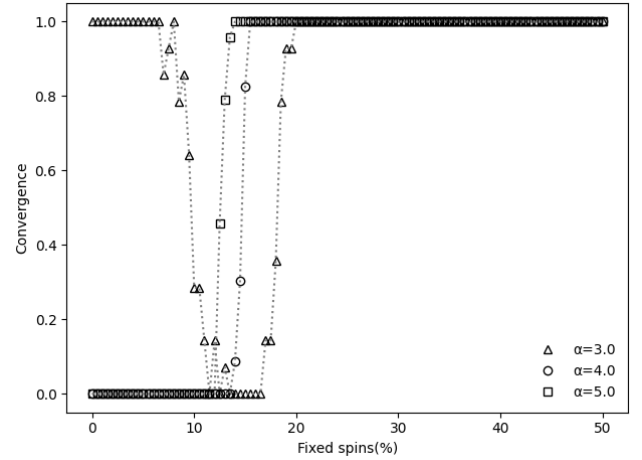


Figure 5. BP convergence probability as a function of the percentage of spins fixed towards a planted solution. Each point corresponds to the average of 30 BP runs on formulas with size $N = 10^4$ at temperature $T = 0.1$.

IV.2. 3-SAT

The K-SAT problem belongs to the NP-complete class. In particular, when defined over random graphs with $K = 3$, it is well known that BP with random initialization fails to converge above $\alpha_d = 3.86$ [3]. However, this is not necessarily the case for the planted ensemble of graphs, where the situation is more complex. In Fig. 5, we show how an informed initialization in planted instances changes the algorithm convergence. For $\alpha = 3$, below the convergence threshold $\alpha_d = 3.86$ of the ensemble of Poisson graphs, we can see that after fixing a few spins ($\phi < 10\%$) towards the planted solution, the convergence is unaffected. However, when the fraction of fixed variables passes $\phi \sim 10\%$ BP stops converging. We find a whole interval where the algorithm does not converge, that for $\alpha = 3$ extends from $\phi \approx 10\%$ to $\phi \approx 20\%$.

For $\alpha > \alpha_d$, instead, BP loses convergence also for small values of ϕ . Only when enough variables are fixed in the direction of the planted solution, we see that BP starts converging. This happens abruptly at a given value of ϕ ($\phi \approx 15\%$ for $\alpha = 4$ and $\phi \approx 12\%$ for $\alpha = 5$), in a behavior reminiscent of what we observed for the 3-XORSAT problem in Figs. 2, 3, and 4.

As said above, in the absence of fixed variables BP fails to converge for $\alpha > \alpha_d$ [3]. Thus, it is not surprising that BP converges for $\alpha = 3$ when $\phi = 0$, while it does not converge for $\alpha = 4$ and $\alpha = 5$ (see Fig. 5). However, the abrupt ascent observed when ϕ is large enough for all three values of α , and the non-monotonicity displayed for $\alpha = 3$, are non-trivial behaviors that we should discuss in more detail.

As identified in Ref. [14] and verified by us in the case of 3-XORSAT with homogeneous connectivity, fixing variables makes BP follow logical implications and effectively assign other variables, in analogy to the Unit Clause Propagation (UCP) algorithm. When the initial fraction of fixed variables ϕ exceeds a critical value ϕ_c , the final fraction of assigned variables $\theta(t^*)$ increases abruptly from a finite value to $\theta(t^*) \sim 1$. Once the assigned variables are removed, we are left with a trivialized constraint satisfaction problem for the remaining part of the system, and BP is able to converge. The latter is possible because the variables are set exactly to their value in the planted solution, avoiding the creation of local contradictions and causing the final ascent that we see for all values of α in Fig. 5.

While for $\alpha = 4$ and $\alpha = 5$ the ascent is the only relevant feature, for $\alpha = 3$ we first have a descent in the probability of convergence. The authors of Ref. [14] demonstrate, for the 3-XORSAT problem, that a large enough fraction ϕ of fixed variables can lead to a remaining constraint satisfaction problem that is inside the clustered phase, even though the solutions of the original problem were not clustered. In other words, it is possible to depart from some $\alpha < \alpha_d$ where the problem is easy to solve (and BP converges), and start fixing variables to a point where the remaining formula is effectively much harder to solve (and BP stops converging). Contradictions will arise because of the presence of cycles in the subjacent hypergraph, and BP's messages will oscillate indefinitely. Nevertheless, if we keep fixing new variables, at some ϕ_c the final fraction of assigned variables jumps to $\theta(t^*) \sim 1$ and the problem becomes easy once more. Thus, BP converges again. This is a plausible explanation for the non-monotonicity of the probability of convergence that we observe for $\alpha = 3$ in Fig. 5.

In Fig. 6, we present the energy (after convergence) for MC as a function of ϕ for different values of α . Notice that this algorithm recovers the ground state of the system only when ϕ is very large. Moreover, the curve is not monotonic. As with the 3-XORSAT in the top panel of Fig. 3, the energy first grows when ϕ is increased. However, once a certain number is fixed, the system begins recognizing the planted solution of the instance.

BP, on the other hand, needs a smaller fraction of fixed variables to find the planted solution. To show it, we plot the overlap defined as before (Fig. 7) as a function of ϕ , both for BP and for MC final configurations. Noticing that BP does not always converge, we include in Fig. 7 only the statistics obtained over the instances where BP converged. We observe again two different behaviors depending on the value of α . For $\alpha < \alpha_d$ ($\alpha = 2$ and $\alpha = 3$ in the figure), BP converges for small values of ϕ , but the final overlap with the planted solution is

small. Once BP regains convergence for larger values of ϕ , it finds probability distributions that have a high overlap with the planted solution.

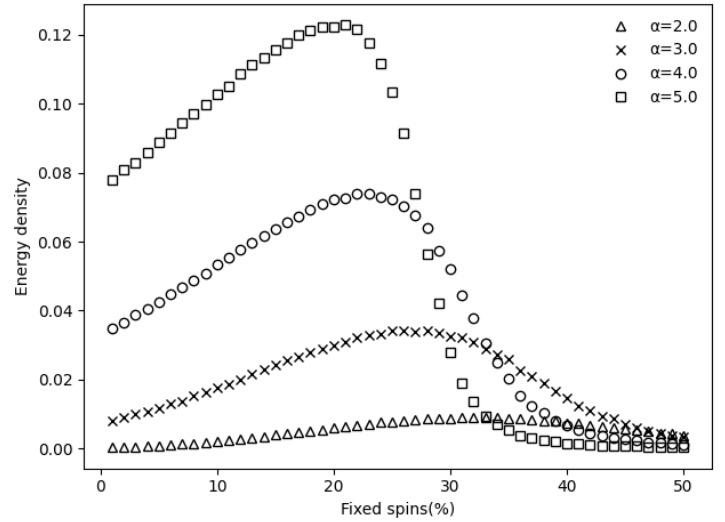


Figure 6. Intensive energy of the final configurations obtained by running MC on random 3-SAT instances as a function of the percentage of fixed spins. The variables are fixed towards a planted solution. The points represent the average of 100 MC runs over formulas of size $N = 1024$ at temperature $T = 0.1$.

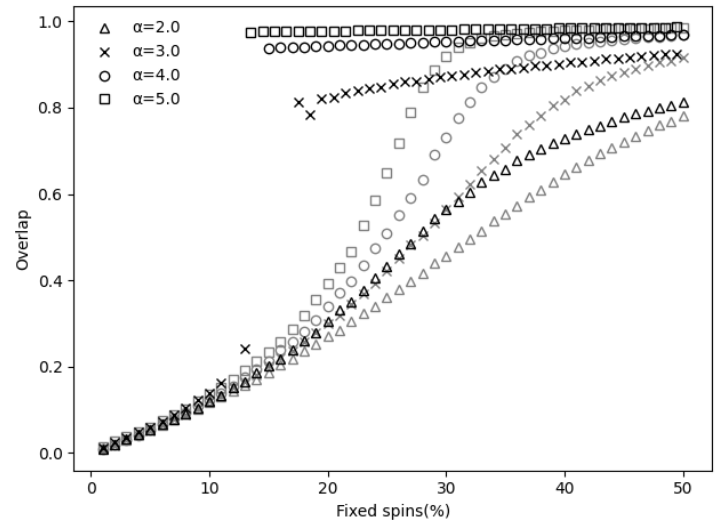


Figure 7. Overlap with the planted solution as a function of the percentage of fixed spins in the 3-SAT problem with $N = 10^4$ at temperature $T = 0.1$. Gray points represent the results of MC, and black points those of BP. The variables are fixed towards the planted solution. Each point represents the average of 20 BP algorithm runs (100 MC runs).

For $\alpha > \alpha_d$, as said before, BP does not converge for small ϕ . However, as soon as it starts converging, the overlap with the planted configuration is close to one. The overlap increases when α increases, as expected in the inference problem. Thus, our results show that running BP with an informed initialization serves two purposes simultaneously: it helps convergence and it drives BP towards the planted solution.

Moreover, the planted solution always has a larger overlap

with the probability densities of BP than with the MC final configurations. The number of fixed spins needed by MC to find the solution is, in any case, much larger than the number of spins needed by BP. For example, when $\alpha = 4.0$ we see that MC starts having overlap close to one around $\phi \approx 40\%$, while BP has comparable overlaps already at $\phi \approx 15\%$.

V. CONCLUSIONS

Our results show that BP is more efficient than MC in finding solutions with an informed initialization. Both for 3-XORSAT and 3-SAT, BP requires a smaller proportion of fixed spins to find the planted solution. Even when the spins are fixed towards random directions, the final configurations obtained from BP for 3-XORSAT instances have low energies. This method could then be used as a starting point to find near-optimal configurations. Furthermore, using an informed initialization helps BP to converge in the planted 3-SAT, in regions where otherwise it would not achieve convergence.

Moreover, we have shown that the behavior of BP when run on 3-XORSAT instances can be accurately reproduced using UCP, a simple algorithm whose analytic description was already included in Ref. [14]. Here, we extended the equations to consider random regular hypergraphs, and show that the fundamental mechanism followed by BP with an informed initialization is the same included in the definition of UCP. Taking advantage that a warm start is given, with a fraction of variables fixed, the algorithm propagates logical implications throughout the graph by assigning the variables that belong to clauses with other $K - 1$ already assigned variables.

Regarding 3-SAT, one should recall the close relation between the $1/4$ model that we used to plant solutions, and the 3-XORSAT problem [29]. Indeed, in this specific case, the planted instances can be transformed into equivalent instances of 3-XORSAT. Thus, it is not surprising that we observe qualitative similarities between both scenarios. However, it must be said that the local algorithms, BP and MC, are not informed that such a transformation exists. If they exploit it in any way, it would be an interesting phenomenon to be investigated in future work.

REFERENCES

- [1] R. Dorfman, P. A. Samuelson, and R. M. Solow, *Linear programming and economic analysis*, international student ed. (McGraw-Hill Kogakusha, New York, 1958).
- [2] S. Cook, in *Proceedings of the 3rd Annual ACM Symposium on Theory of Computing* (ACM, New York, 1971), p. 151.
- [3] M. Mezard and A. Montanari, *Information, physics, and computation* (Oxford University Press, Oxford, 2009).
- [4] M. Mezard, G. Parisi, and R. Zecchina, *Science* **297**, 812 (2002).
- [5] F. Krzakala, A. Montanari, F. Ricci-Tersenghi, and L. Zdeborova, *Proc. Natl. Acad. Sci.* **104**, 10319 (2007).
- [6] M. Alava, J. Ardelius, E. Aurell, P. Kaski, S. Krishnamurthy, P. Orponen, and S. Seitz, *Proc. Natl. Acad. Sci.* **105**, 15253 (2008).
- [7] D. Achlioptas and A. Coja-Oghlan, in *2008 49th Annual IEEE Symposium on Foundations of Computer Science* (IEEE, New York, 2008), pp. 793-802.
- [8] E. Aurell, E. Domínguez, D. Machado, and R. Mulet, *Phys. Rev. Lett.* **123**, 230602 (2019).
- [9] C. H. Papadimitriou, in *Proceedings of the 32nd IEEE Symposium on the Foundations of Computer Science* (IEEE Computer Society, New York, 1991), pp. 163-169.
- [10] E. Aurell, U. Gordon, and S. Kirkpatrick, in *Advances in Neural Information Processing Systems*, Vol. 17, edited by L. Saul, Y. Weiss, and L. Bottou (MIT Press, Cambridge, 2004).
- [11] S. Seitz, M. Alava, and P. Orponen, *J. Stat. Mech. Theory Exp.* **2005**, P06006 (2005).
- [12] S. Kirkpatrick, C. D. Gelatt, and M. P. Vecchi, *Science* **220**, 671 (1983).
- [13] M. C. Angelini and F. Ricci-Tersenghi, *Phys. Rev. X* **13**, 021011 (2023).
- [14] F. Ricci-Tersenghi and G. Semerjian, *J. Stat. Mech. Theory Exp.* **2009**, P09001 (2009).
- [15] L. Budzynski, F. Ricci-Tersenghi, and G. Semerjian, *J. Stat. Mech. Theory Exp.* **2019**, 023302 (2019).
- [16] F. Ricci-Tersenghi, M. Weigt, and R. Zecchina, *Phys. Rev. E* **63**, 026702 (2001).
- [17] S. Franz, M. Leone, F. Ricci-Tersenghi, and R. Zecchina, *Phys. Rev. Lett.* **87**, 127209 (2001).
- [18] A. Montanari and F. Ricci-Tersenghi, *Phys. Rev. B* **70**, 134406 (2004).
- [19] M. Bellitti, F. Ricci-Tersenghi, and A. Scardicchio, *Phys. Rev. Res.* **3**, 043015 (2021).
- [20] M. Bernaschi, M. Bisson, M. Fatica, E. Marinari, V. Martin-Mayor, G. Parisi, and F. Ricci-Tersenghi, *Europhys. Lett.* **133**, 60005 (2021).
- [21] S. Mertens, M. Mezard, and R. Zecchina, *Random Struct. Algorithms* **28**, 340 (2006).
- [22] A. Montanari, F. Ricci-Tersenghi, and G. Semerjian, *J. Stat. Mech. Theory Exp.* **2008**, P04004 (2008).
- [23] H. Zhou, *Eur. Phys. J. B* **73**, 617 (2010).
- [24] F. Krzakala and J. Kurchan, *Phys. Rev. E* **76**, 021122 (2007).
- [25] M. C. Angelini and F. Ricci-Tersenghi, *Phys. Rev. E* **100**, 013302 (2019).
- [26] A. G. Cavaliere and F. Ricci-Tersenghi, *J. Stat. Mech. Theory Exp.* **2025**, 053405 (2025).
- [27] D. Gamarnik and M. Sudan, in *Proceedings of the 5th Conference on Innovations in Theoretical Computer Science* (Association for Computing Machinery, New York, 2014), pp. 369-376.
- [28] D. Gamarnik and A. Jagannath, *Ann. Probab.* (2019).
- [29] W. Barthel, A. K. Hartmann, M. Leone, F. Ricci-Tersenghi, M. Weigt, and R. Zecchina, *Phys. Rev. Lett.* **88**, 188701 (2002).
- [30] F. Krzakala and L. Zdeborova, *Phys. Rev. Lett.* **102**, 238701 (2009).
- [31] F. Zamponi, *Mean field theory of spin glasses*, arXiv:1008.4844 (2014).
- [32] N. Metropolis, A. W. Rosenbluth, M. N. Rosenbluth, A. H. Teller, and E. Teller, *J. Chem. Phys.* **21**, 1087 (1953).

- [33] E. Aurell, E. Domínguez, D. Machado, and R. Mulet, Phys. Rev. E **97**, 05103(R) (2018).
[34] E. Aurell, G. Del Ferraro, E. Domínguez, and R. Mulet, Phys. Rev. E **95**, 052119 (2017).
[35] E. Domínguez, D. Machado, and R. Mulet, J. Stat. Mech. Theory Exp. **2020**, 073304 (2020).
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MATHEMATICAL MODEL FOR ESTIMATING SOIL REDISTRIBUTION RATE BY WATER EROSION USING THE NUCLEAR AND ISOTOPIC FRN TECHNIQUE

MODELO MATEMÁTICO PARA ESTIMAR LA TASA DE REDISTRIBUCIÓN DEL SUELO POR EROSIÓN HÍDRICA UTILIZANDO LA TÉCNICA NUCLEAR E ISOTÓPICA FRN

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The use of nuclear techniques for the evaluation of soil water erosion is based on empirical relations to evaluate inventories of radionuclides in the soil (^{137}Cs , ^{210}Pb and ^7Be). In applying the fallout radionuclides technique (FRN) to croplands, the most widely used model is the Mass Balance Model (MBM-II), which employs ^{137}Cs isotope inventories (Bq m^{-2}) to estimate soil redistribution rate. This work develops a mathematical model (MRS-2) to obtain this soil redistribution rate, yielding results comparable to those of MBM-II. The model estimates the soil redistribution rate based on areal activity density (AAD) values (Bq m^{-2}) used in FRN techniques. This linear model is notable for its internal and external validation, providing reliable estimates of soil redistribution rate down to values of $-60 \text{ t ha}^{-1} \text{ y}^{-1}$. Its use is therefore recommended.

El uso de técnicas nucleares para evaluar la erosión hídrica del suelo se fundamenta en el establecimiento de relaciones empíricas para evaluar los inventarios de radionucleidos en el suelo (^{137}Cs , ^{210}Pb y ^7Be). Al aplicar la técnica de radionucleidos de precipitaciones (FRN) a las tierras cultivadas, el modelo más utilizado es el Balance de Masa (MBM-II), que emplea inventarios de isótopo ^{137}Cs (Bq m^{-2}) para estimar la tasa de redistribución del suelo. Este trabajo desarrolla un modelo matemático (MRS-2) para obtener esta tasa de redistribución del suelo, produciendo resultados comparables a los del modelo MBM-II. El modelo estima la tasa de redistribución basándose en valores de densidad superficial de actividad (DSA, en Bq m^{-2}) utilizados en la técnica FRN. Este modelo lineal es notable por su validación interna y externa, proporcionando estimaciones fiables de la tasa de redistribución del suelo hasta $-60 \text{ t ha}^{-1} \text{ y}^{-1}$. Por lo tanto, se recomienda su uso.

Keywords: water erosion (erosión hídrica), fallout radionuclides (radionúclidos de precipitación), soil redistribution (redistribución del suelo), conversion model (modelo de conversión)

I. INTRODUCTION

Soil loss due to water erosion and its subsequent sedimentation in the landscape and water reservoirs is a global environmental problem affecting agriculture and hydraulic infrastructure. The negative impacts include threats to agricultural sustainability and water resources, requiring comprehensive assessments using reliable tools such as nuclear techniques [1,2] to characterize soil health [3]. Water erosion, the most common problem, is caused by surface runoff from soil. The nuclear technique (FRN) assesses water erosion directly and quantitatively, as its isotopic tracers move coupled with soil particles transported by water.

Numerous traditional techniques and universal equations exist to estimate soil loss, such as USLE [4], RUSLE [5], and MUSLE [6]. Their use, combined with the Geographic Information System (GIS), is widespread [7]. Additional model estimates redistribution in cultivated soils [8] and evaluates the effect of crop rotation and land-use changes on sediment transport [9]. Compared to these models, practical experience with nuclear and isotopic techniques has significant advantages by overcoming their limitations,

moving beyond predictive frameworks to deliver more precise and concrete results.

A key advancement is the use of fallout radionuclides (FRN) to evaluate soil redistribution rate [10–12]. This technique uses the artificial anthropogenic isotope from nuclear explosions (^{137}Cs), the natural cosmogenic isotope (^7Be), and the natural geogenic isotope (^{210}Pb) to define erosion and sedimentation zones. These radionuclides provide information on soil redistribution across different time scales: ^7Be (several months) [13], ^{137}Cs (approximately 50 years) [14,15], and ^{210}Pb (approximately 100 years) [16]. The IAEA has been actively involved in developing these nuclear techniques [17,18].

To convert ^{137}Cs inventories into soil erosion/deposition rates, software has been developed as a standard add-in for Microsoft Excel. These models are complex and tedious, involving an evaluation process based on laboratory-derived mass activity density (MAD-Bq kg^{-1}). For ^{137}Cs , temporal variation is assessed using the traditional conversion Mass Balance Model II (MBM-II), which accounts for time-varying ^{137}Cs inputs and the fate of newly deposited precipitation before its incorporation into the plow layer. Currently, FRNs

enable the evaluation of erosion processes and extreme climatic events [19] and have been used as tracers in aquatic systems to indicate sediment residence times and to identify their sources [20,21].

The main objective of this work was to obtain, develop, and validate a mathematical model that would allow for the evaluation of soil redistribution per unit area in a shorter time, thereby improving the efficiency of the assessment process in the short and medium term and providing a practical replacement for the lengthy traditional calculation methods.

II. MATERIALS AND METHODS

The use of fallout radionuclides (FRN) to assess water erosion is based on the conversion models that consider radionuclide inventories in the soil (¹³⁷Cs, ²¹⁰Pb, and ⁷Be) to estimate soil redistribution rate [7–9,16,22].

Radionuclide measurements were performed using a hyperpure germanium gamma spectrometer with 35 % efficiency. The expanded uncertainty ranged from ±0.13 to ±8.24, determined by multiplying the combined standard uncertainty by a cover factor. The stability of the gamma spectrometer system was monitored weekly by measuring energy, resolution, and efficiency values for point sources of Am-²⁴¹ (59.54 keV), Cs-¹³⁷ (661.66 keV), and Co-60 (1332.50 keV), as well as the background count rate across the entire analytical range. The Monte Carlo statistical simulation was used to accurately solve the measurement problem [22], and the system remained stable throughout the sampling process. The activity concentrations for the radionuclides in the IAEA-300, IAEA-306, and IAEA-314 certified reference materials were determined. The measurement results were compared with target values, revealing no significant differences.

The results of this work led to a new mathematical model (MRS-2) for estimating soil redistribution rate based on areal activity density (AAD) values (Bq m⁻²) and other factors used in the FRN technique, as part of the integrated methodology of the nuclear techniques [1,2]. This model is less complex, yielding results more quickly from AAD values and making the evaluation process more efficient in the short and medium term. It practically eliminates the need for a reference site. The development of the MRS-2 model is based on results from previous research involving 151 samples from the studied sites in the Hanabanilla reservoir and the National Site for the Conservation of Water, Soil, and Forests (Havana). Soil sampling followed expert criteria and a combination of random, stratified, and systematic protocols [12,17]. Detailed knowledge of the study areas and the use of composite sampling prevented cross-contamination.

II.1. The methodological strategy used is described below:

- 1) Analysis of bivariate correlations between the following variables: areal activity density (AAD, Bq m⁻²), soil

redistribution rate (t ha⁻¹ y⁻¹), soil density (kg cm⁻³), geology, soil type and use, height (m), rainfall (mm), soil moisture, and soil slope (%).

- 2) Hierarchical classification analysis of all variables involved to determine their grouping based on results similarity.
- 3) Selection of the variable(s) with the highest correlation linked to the dependent variable (soil redistribution rate (t ha⁻¹ y⁻¹)).
- 4) Analysis of bivariate model fits related to the dependent variable (soil redistribution rate (t ha⁻¹ y⁻¹)).
- 5) Internal validation of the model based on data from the study region and external validation in the National Site for Soil, Water, and Forest Conservation, located in Havana Province. In this area, soil redistribution results from applying the integrated methodology were analyzed using 50 sample sites and statistically compared with the results estimated by the model, using the Kolmogorov-Smirnov statistical test to compare two distributions and the mean absolute error.
- 6) External validation through the application of the integrated methodology, culminating in results graphs and thematic maps. All statistical analyses for obtaining, evaluating, and validating the linear model were performed using the software Statgraphics Centurion (version 19.5.01).

III. RESULTS AND DISCUSSION

Bivariate correlation analysis among the studied variables revealed only one high and significant correlation: between areal activity density (Bq m⁻²) and soil redistribution (t ha⁻¹ y⁻¹), with a coefficient of 0.956. The remaining variables showed no significant influence on soil redistribution rate (see Table 1).

Hierarchical classification analysis showed a cluster formed by the AAD and the calculated soil redistribution rate, clearly separated by their Euclidean distances from the other variables. This confirms the bivariate correlation results, where both variables exhibited the strongest correlation (above 95 %).

Table 1. Results of the bivariate correlation analysis for all studied variables.

¹Soil redistribution rate

Studied variables	Correlation coefficients	
	AAD (Bq m ⁻²)	SRR ¹ (t ha ⁻¹ yr ⁻¹)
AAD (Bq m ⁻²)	—	0.9557
SRR (t ha ⁻¹ yr ⁻¹)	0.9557	—
Soil density (kg cm ⁻³)	0.1230	0.1573
Geology	-0.0057	-0.0740
Land use	0.1927	0.2807
Soil type	-0.0798	-0.0865
Height (m)	0.4139	0.4942
Rainfall (mm)	0.3560	0.4005
Soil moisture index	-0.1709	-0.1747
Soil slope (%)	0.3123	0.3585

Based on these results, linear regression models were analyzed to select the optimal model for estimating soil redistribution rate from AAD values derived from laboratory mass activity density (MAD, Bq kg⁻¹) values.

The AAD (Bq m⁻²) is the selected parameter for the model and is the main input for most conversion models applied in FRN. It is calculated as follows:

$$AAD = \frac{M \cdot MAD}{S} \quad (1)$$

where M is the total mass of whole soil core in kg, MAD is the mass activity density (Bq kg⁻¹) and S is the area of the core cross-section (m²).

Simple linear regression analysis was performed. The best fit was obtained with a linear regression model using the square root of the areal activity density ($\sqrt{AAD}$) as the independent variable. The results are shown in Tables 2 and 3 and Fig. 1.

Table 2. Model coefficients.

Parameter	Least Squares Estimate	Standard Error	T Statistic	P-value
Intercept	-83.0182	1.40182	-59.2216	0.0000
Slope	2.71585	0.0399165	68.0683	0.0000

Table 3. Analysis of Variance..

Source	Sum of Squares	Df	Mean Square	F-Ratio	P-value
Model	216814	1	216814	4629.21	0.0000
Residual	6978.58	149	46.8361		
Total (Corr.)	223793	150			

- Correlation coefficient = 0.9843
- R-squared = 96.8817 %
- R-squared (adjusted for d.f.) = 96.8607 %
- Standard error of the estimate = 6.8437
- Mean absolute error = 5.5039

- Durbin-Watson statistic = 1.8739 ($P = 0.2202$)
- Autocorrelation of residuals at lag 1 = 0.0602

The equation of the fitted model (MRS-2) is:

$$SR (t ha^{-1} y^{-1}) = -83.0182 + 2.71585 \sqrt{AAD} (Bq m^{-2}) \quad (2)$$

- SR: Soil redistribution

The P-value in the ANOVA Table (< 0.05) indicates a statistically significant relationship between the calculated soil redistribution and the AAD (Bq m⁻²) at the 95.0 % confidence level. The fitted model explains 96.86 % of the variability in the calculated soil redistribution. The correlation coefficient of 0.9843 indicates a strong relationship between the variables.

Applying the linear model obtained from linear regression analysis with the ($\sqrt{AAD}$), soil redistribution values were estimated and compared with those calculated using MBM-II to determine deviations. The mean absolute error was 5.003 t ha⁻¹ y⁻¹. This value is acceptable for the proposed model, which estimates soil redistribution rates up to 60 t ha⁻¹ y⁻¹, considering that loss levels up to approximately 7 t ha⁻¹ y⁻¹ are classified as low erosion levels.

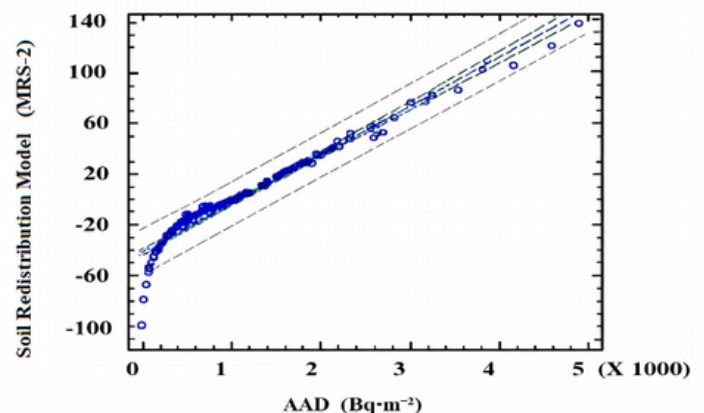


Figure 1. Calculated soil redistribution rate and its dependence on AAD (Bq m⁻²).

The Kolmogorov-Smirnov test was used to compare both distributions. The results are shown below:

- Sample 1: Soil redistribution MBM II model (t ha⁻¹ y⁻¹)
- Sample 2: Redistribution MRS-2 model (t ha⁻¹ y⁻¹)

Kolmogorov-Smirnov Test:

- Statistic DN estimated = 0.0861
- Two-tailed K-S statistic for large samples = 0.7481
- Approximate P-values = 0.6304

In this case, the maximum distance is 0.0861 (visible in the Quantile Plot, Fig. 2). As the P-value is ≥ 0.05 , there is no statistically significant difference between the two distributions, demonstrating the model's internal validity. However, this result needs to be complemented with its geographical expression of the territorial conditions where the variables studied in the correlational analysis are present.

Fig. 2 shows a close approximation between the two distributions. However, estimated soil redistribution rates below $-60 \text{ t ha}^{-1} \text{ y}^{-1}$ begin to diverge from calculated values. The MRS-2 model provides optimal results up to the erosion range of $-60 \text{ t ha}^{-1} \text{ y}^{-1}$. High soil loss values correspond to very low concentrations of the studied radionuclide (^{137}Cs) in soil samples (values close to the detection limit of gamma-ray spectrometry), leading to greater uncertainty in the estimated analytical values for the mass activity density (Bq kg^{-1}). This error propagates when calculating the main model variable, areal activity density (Bq m^{-2}), which is used to estimate soil redistribution ($\text{t ha}^{-1} \text{ y}^{-1}$).

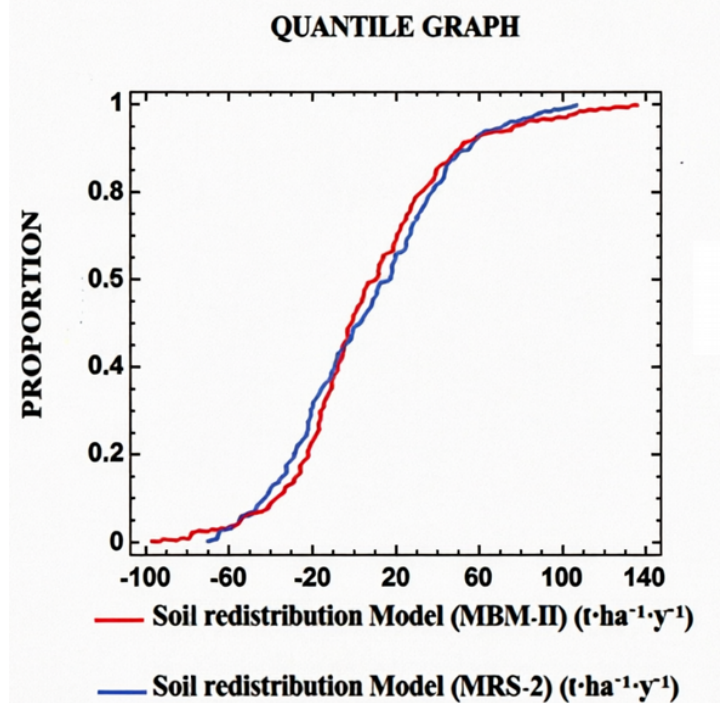


Figure 2. Comparison of calculated soil redistribution rate and soil redistribution rate estimated by the MSR-2 model

III.1. Practical application of the MRS-2 model in case studies.

The MRS-2 mathematical model is validated statistically and practically. The statistical analyses are presented above; practical validation is demonstrated through various case studies. Below is a comparison of soil redistribution results obtained by applying the traditional conversion model (MBM-II) and the new mathematical model (MRS-2). Both models were applied in the following study areas: crop fields in the Provincial site for Soil, Water, and Forest Conservation

(Cienfuegos) and the Hanabanilla Reservoir (Cienfuegos and Villa Clara).

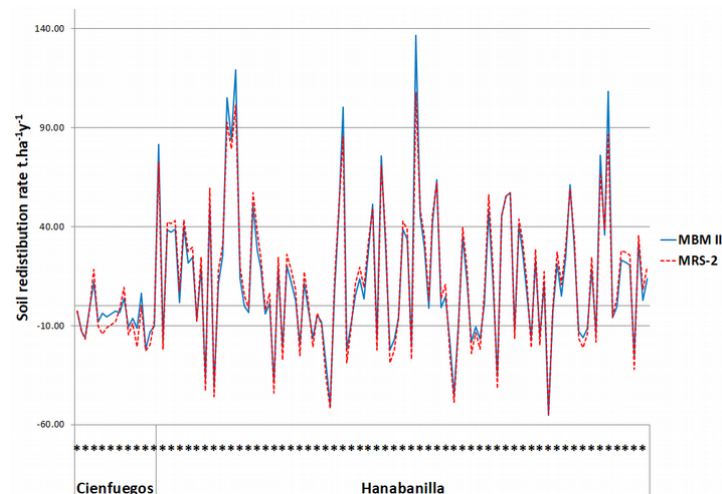


Figure 3. Comparison of soil redistribution estimates from the linear model obtained (MRS-2) with the MBM-II. Internal validation.

The research enabled the assessment of soil redistribution in the landscape and the reservoir through the application of both models. To validate the efficiency of the MRS-2 model, its results are compared with those from the traditional MBM-II model using GIS (QGIS, version 3.22.6) for mapping and OpenOffice (version 4.1.7) for graphics (see Fig. 3).

III.2. Validation of the mathematical model (MRS-2).

III.2.1. Results (Hanabanilla Sub-Basin).

The conversion models (MBM-II and MRS-2) were applied in the basin of the Hanabanilla Reservoir in Cienfuegos. The main land uses in the study site are forestry, coffee, livestock, and seasonal crops. The interpolation (kriging) results for 115 points are shown in figures 4A (MBM-II) and 4B (MRS-2). The areas of soil gain (positive values) and loss (negative values) are clearly identified. The same color palette was used for both models for comparison.

The Fig. 4A show the MBM-II model estimates a soil redistribution range from -43 to $119 \text{ t ha}^{-1} \text{ y}^{-1}$. The MRS-2 model (Fig. 4B) estimates a range of soil redistribution values from -60 to $118 \text{ t ha}^{-1} \text{ y}^{-1}$, very similar to the MBM-II, reflected in the proximity of the spatial redistribution pattern. The distribution of positive and negative values on the map shows a high coincidence, as do the soil redistribution rates isolines. Analysis of the residuals ($\text{t ha}^{-1} \text{ y}^{-1}$) between model's prediction shows a mean (-0.4) and standard error (0.6) close to zero, indicating the closeness of both models. This confirms the internal validation from the Kolmogorov-Smirnov test.

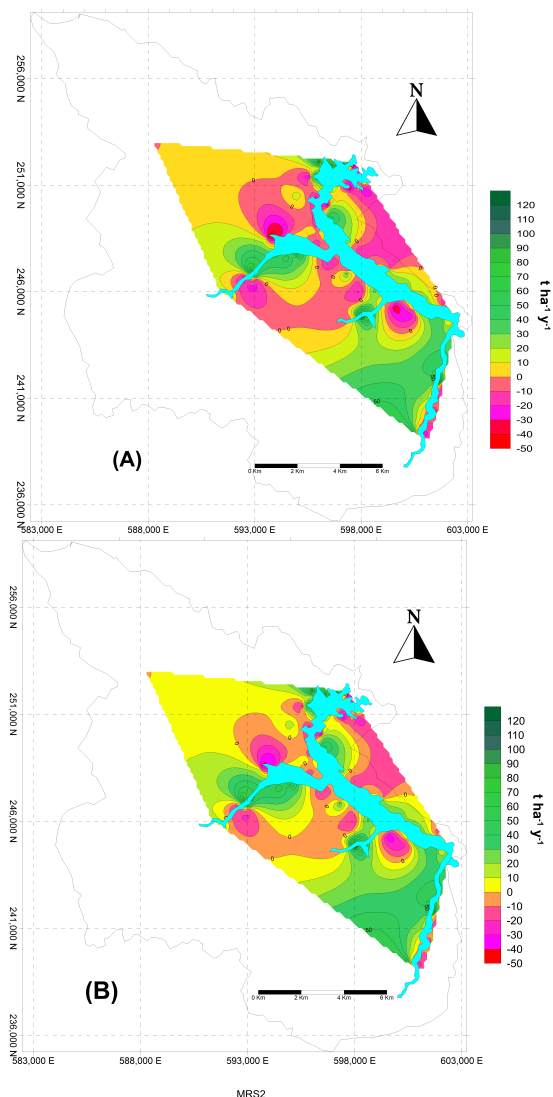


Figure 4. Interpolation results of the (A) MBM-II model and (B) MRS-2 model in Hanabánilla areas.

III.3. External validation of the model obtained

Crop fields in the National Site for Soil, Water, and Forest Conservation (Havana Province) were used for the external validation of the MSR-2 model. The model behaves similarly to the MBM-II model, following the pattern of maximum and minimum soil redistribution estimates. Differences appear for high erosion loss levels exceeding $-60 \text{ t ha}^{-1} \text{ y}^{-1}$. The MRS-2 model adequately fits the MBM-II results at most evaluated points.

The study site is highly eroded, as represented in Fig. 5A for the ^{137}Cs study. The main land uses are livestock and seasonal crops. The majority of the area shows negative redistribution rates (soil losses) with values below $-15 \text{ t ha}^{-1} \text{ y}^{-1}$; only a small green strip (center) identifies areas with tolerable soil loss levels ($-10 \text{ t ha}^{-1} \text{ y}^{-1}$). Three areas with very high erosion levels are shown in orange to red bands in the southwest, south, and northeast of the site.

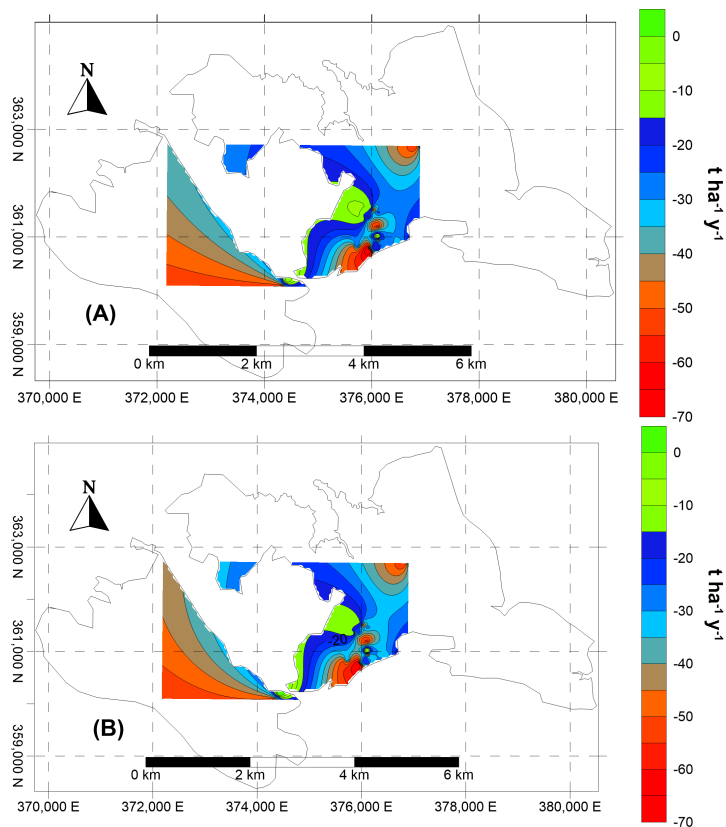


Figure 5. Interpolation results of the (A) MBM-II model and (B) MRS-2 model in the national site.

For comparison, MRS-2 results in the same national site areas were mapped using the kriging interpolation technique with the same soil redistribution values scale as MBM-II (Fig. 5B). This linear model shows results close to the reference model, and the spatial distribution shows very similar soil redistribution isolines. Residuals ($\text{t ha}^{-1} \text{ y}^{-1}$) between model predictions have a low mean (1.2) and a standard error (0.03) close to zero, demonstrating the proximity of both models for assessment.

This comparative analysis confirms the statistical results and establishes greater confidence in the MRS-2 model. Fig. 6 illustrates the impact of these differences between the models when evaluating their spatial representation, a fundamental step in interpreting FRN technique results.

The external validation was conducted at the national site on transects across several plots with diverse conservation measurements. Results are shown in Table IV.

Table 4. Comparison of soil redistribution models

Redistribution Models.	Sample 1 (MBM-II)	Sample 2 (MRS-2)
Real Soil redistribution (national site)	50 values (-61.81 to 18.22)	-
Soil Redistribution of (Linear model MRS-2)	-	50 values (-59.0146 to 23.7892)

Kolmogorov-Smirnov Test:

- Estimated DN statistic = 0.2
- Two-tailed K-S Statistic for large samples = 1.0
- Approximate P-value = 0.2710

In this case, the maximum distance is 0.2 (Fig. 6, Quantile Plot). As the P-value is > 0.05 , there is no statistically significant difference between the two distributions at 95.0 % confidence levels (Fig. 7).

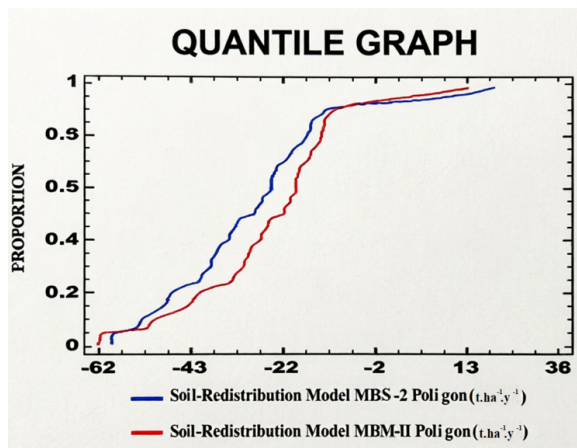


Figure 6. Comparison of soil redistribution rates: calculated (MBM II) vs. obtained by the MSR-2 model at national test site.

At the national site, all soil redistribution values are negative, representing different soil loss levels. The linear model shows the same behavior as the MBM-II model for the different points evaluated (Fig. 7). The closest values between models are for estimates above $-50 \text{ t ha}^{-1} \text{ y}^{-1}$. Beyond $-60 \text{ t ha}^{-1} \text{ y}^{-1}$ (maximum soil loss values), the models show the greatest differences.

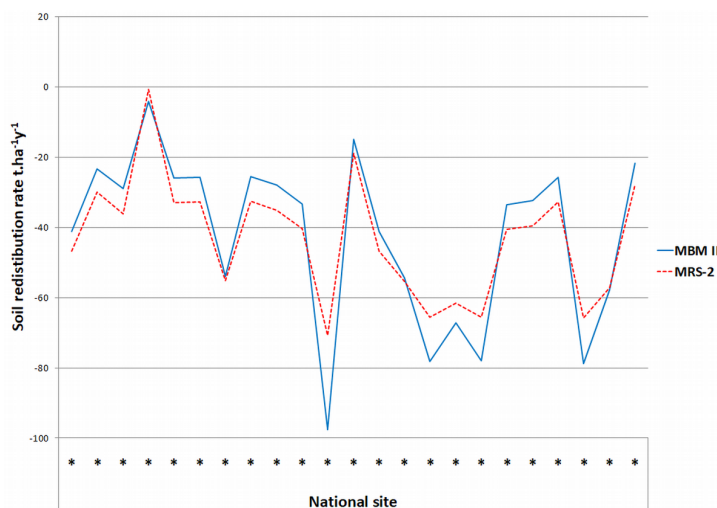


Figure 7. Comparison of soil redistribution estimates from the linear model (MRS-2) with the MBM-II model. External validation.

III.4. Potentials for practical application of the mathematical model (MRS-2).

Considering the stated premises, advantageous background, and the statistical behavior of the MRS-2 model, its application is proposed as a tool for estimating soil redistribution rates in landscape and water reservoirs. Its results exhibit a very good approximation with the traditional Conversion Model (particularly MBM-II), except where the erosion exceeds $-60 \text{ t ha}^{-1} \text{ y}^{-1}$. Applying this linear model simplifies the use of FRN techniques by eliminating the need to define and measure a reference site. This is particularly useful where defining a reference site to estimate reference AAD is not possible.

The application potential of the mathematical model MRS-2 is high. Applying a modified version of the Universal Soil Loss Equation (RUSLE) to estimate soil loss across the European Union (study area: $3941 \times 103 \text{ km}^2$), with an emphasis on cultivated soils, identified that over 99 % of the assessed area falls within the range of 0 to $-50 \text{ t ha}^{-1} \text{ y}^{-1}$. This indicates the MRS-2 model could have potential use throughout this region. A study in northeast Ethiopia using Geographic Information Systems (GIS) and remote sensing techniques (RUSLE) classified soil erosion risk from low ($0 - 7 \text{ t ha}^{-1} \text{ y}^{-1}$) to severe ($45 - 60 \text{ t ha}^{-1} \text{ y}^{-1}$) and very severe ($> 60 \text{ t ha}^{-1} \text{ y}^{-1}$). Results showed that 98 % of the total studied area was in the $0 - 60 \text{ t ha}^{-1} \text{ y}^{-1}$ range, again confirming the potential use of the MRS-2 model from low to severe erosion levels (according to this classification).

IV. CONCLUSION

- The MRS-2 linear mathematical model simplifies soil redistribution estimations using areal activity density (AAD) and can replace complex traditional methods during initial screening.
- Its reliability and applicability have been demonstrated in diverse landscape contexts and agroecosystems and verified using maps, graphs, and case studies.

V. ACKNOWLEDGEMENT

The authors acknowledge the work carried out by the International Atomic Energy Agency (IAEA), through the Joint Division with the Food and Agriculture Organization (FAO), in assisting Member States to apply nuclear techniques to address challenges in food safety and sustainable agricultural development.

V.1. Data availability

The authors are willing to provide the database used to generate the MRS-2 code upon reasonable request. Access is granted solely for the purpose of reproducing or validating the results reported in this study. Any other use of the data requires prior authorization from the authors.

REFERENCES

- [1] J. L. Peralta Vital, R. H. Gil Castillo, Y. Llerena Padrón, Y. M. Cordoví Miranda, N. Labrada Arevalo, and L. Alonso Pino, *Int. Soil Water Conserv. Res.* **8**, 406 (2020).
- [2] J. L. Peralta Vital, L. E. Calvo Gobbetti, Y. Llerena Padrón, F. H. Martínez Luzardo, O. Díaz Rizo, and R. Gil Castillo, *Appl. Sci.* **14**, 9189 (2024).
- [3] Z. Hussain, L. Deng, X. Wang, R. Cui, and G. Liu, *Sustainability* **14**, 9300 (2022).
- [4] J. Li, M. Xiong, R. Sun, and L. Chen, *Int. Soil Water Conserv. Res.* **12**, 1 (2024).
- [5] K. Ghosal and S. Das Bhattacharya, *J. Indian Soc. Remote Sens.* **48**, 689 (2020).
- [6] R. Benavidez, B. Jackson, D. Maxwell, and K. Norton, *Hydrol. Earth Syst. Sci.* **22**, 6059 (2018).
- [7] R. S. Padala and A. J. Mathew, *Water Clim. Change* **15**, 3138 (2024).
- [8] J. Soto and A. Navas, *Radiat. Meas.* **43**, 1285 (2008).
- [9] I. L. Villuendas, B. Latorre, L. Gaspar, and A. Navas, *Hydrol. Processes* **36**, e14577 (2022).
- [10] M. Cabrera, R. Sanabria, J. González, P. Cabral, S. Tejeda, Z. Graciela, and M. Tassano, *Geoderma* **435**, 116502 (2023).
- [11] FAO, The state of the world's land and water resources for food and agriculture: Systems at breaking point (FAO, Rome, 2021)(<https://doi.org/10.4060/cb7654es>).
- [12] Y. Llerena Padrón, R. Gil Castillo, J. L. Peralta Vital, Y. Cordoví Miranda, L. Bravo Leyva, and A. Fuentes Soto, *Nucleus* **72** (2022).
- [13] S. Kumar, A. D. Raj, and S. Mariappan, *Catena* **234**, 107591 (2024).
- [14] K. Haejin, O. K. Kyeong, K. Sang-Yeob, S. Kyung-Suk, and K. Kyonghwan, *Mar. Pollut. Bull.* **212**, 117562 (2025).
- [15] J. M. Abril-Hernández, *J. Mar. Sci. Eng.* **13**, 144 (2025).
- [16] IAEA, IAEA and FAO Celebrate 60-Year Milestone in Advancing Nuclear Techniques for Agriculture (2024) (<https://www.iaea.org/newscenter/news/iaea-and-fao-celebrate-60-year-milestone-in-advancing-nuclear-techniques-for-agriculture>).
- [17] F. Zapata, E. Garcia-Agudo, J. C. Ritchie, and P. G. Appleby, *Handbook for the assessment of soil erosion and sedimentation using environmental radionuclides* (Kluwer Academic, Dordrecht, 2003).
- [18] P. Porto, E. Fulajtar, and L. Kheng-Heng, *J. Environ. Sci. Health Part A* (2024).
- [19] E. G. Muñoz-Arcos, G. E. Millward, C. C. Clason, C. M. Bravo-Linares, and W. H. Blake, *Sci. Total Environ.* **959**, 178177 (2025).
- [20] T. Abere, O. Evrard, T. E. Chalaux-Clergue, H. Adgo, E. Lemma, A. Verleyen, and A. Frankl, *J. Soils Sediments* (2025).
- [21] M. F. Habtamu, W. A. Dessalew, M. Louise, H. Amare, A. T. Seifu, B. Jennie, and S. S. Tammo, *Catena* **234**, 107539 (2024).
- [22] G. Eleftheriou, C. Tsabaris, E. G. Androulakaki, F. K. Pappa, and E. G. Patiris, *Appl. Radiat. Isot.* **206**, 111234 (2024).

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COMPUTATIONAL ANALYSIS OF STRUCTURAL STABILITY AND RESISTANCE TO GAMMA AND ELECTRON RADIATION IN LMO AND LNMO SPINELS.

ANÁLISIS COMPUTACIONAL DE LA ESTABILIDAD ESTRUCTURAL Y LA RESISTENCIA A LA RADIACIÓN GAMMA Y ELECTRÓNICA EN ESPINELAS LMO Y LNMO.

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This study investigates the response to gamma and electron radiation of materials used as cathodes in lithium-ion batteries, specifically LiMn_2O_4 (LMO) and $\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4$ (LNMO), through the computational analysis of displacement cross-sections per atom. The results indicate that the partial substitution of Mn with Ni in LNMO significantly increases radiation resistance, which is attributed to the strengthening of Ni-O covalent bonds, the reduction of Jahn-Teller distortions, and the stabilization of the crystal lattice. Monte Carlo simulations using the MCCM software reveal that LNMO requires energies 1.3 – 1.8 times higher for the initiation of atomic displacement cascades compared to LMO.

Este estudio investiga la respuesta a la radiación gamma y electrónica de materiales empleados como cátodo en baterías de iones de litio, específicamente LiMn_2O_4 (LMO) y $\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4$ (LNMO), mediante el análisis computacional de las secciones eficaces de desplazamientos por átomo. Los resultados indican que la sustitución parcial de Mn por Ni en el LNMO incrementa significativamente la resistencia a la radiación, lo cual se atribuye al fortalecimiento de enlaces covalentes Ni-O, la reducción de las distorsiones Jahn-Teller y la estabilización de la red cristalina. Las simulaciones por Monte Carlo usando el software MCCM revelan que el LNMO requiere de energías 1,3 – 1,8 veces mayores para que se dé inicio a las cascadas de desplazamiento atómico en comparación con LMO.

Keywords: spinel materials (materiales de espinela), radiation damage (daño por radiación), threshold displacement energy (energía umbral de desplazamiento), lithium-ion batteries (baterías de iones de litio), atomic displacement cascades (cascadas de desplazamiento atómico)

I. INTRODUCTION

Spinel compounds, characterized by the general formula AB_2O_4 and a robust three-dimensional crystal structure (space group $Fd\bar{3}m$) [1], constitute a critically important class of electrode materials for advanced rechargeable battery systems, particularly lithium-ion batteries (LIBs). Their appeal stems from an advantageous combination of structural stability, high operational voltage, and promising rate capability [2]. The archetypal framework consists of a cubic close-packed (ccp) array of oxide anions (O^{2-}), where the A^{2+} cations occupy one-eighth of the tetrahedral sites (Wyckoff position 8a) and the B^{3+} cations reside in half of the octahedral sites (16d) [3] [4]. In electrochemically active lithium-based spinels (e.g., LiMn_2O_4), the A site is occupied by Li^+ ions, while the B site is filled by transition metal ions (e.g., $\text{Mn}^{3+}/\text{Mn}^{4+}$ or Ni^{2+}), whose redox activity enables lithium (de)intercalation.

This arrangement confers unique properties: high ionic conductivity, thermal stability, and resistance to extreme conditions [5]. The substitution of Mn by Ni in LiMn_2O_4 (LMO) generates $\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4$ (LNMO), altering the cation distribution and modifying electronic interactions, which directly impacts the threshold displacement energy (TDE) [6].

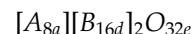
Previously, it has been experimentally demonstrated that

gamma radiation significantly modifies the electrochemical properties of spinel cathodes [7], due to the generation of structural defects. However, the atomic origin of these changes — in particular, the atomic displacements induced by secondary electrons — has not been quantified in LMO and LNMO. Therefore, the present work determines, for each atom and according to its crystallographic position (tetrahedral or octahedral), the probability of atomic displacement and the associated threshold energies, thereby providing a mechanistic explanation for the greater stability of LNMO against radiation.

II. FUNDAMENTALS

II.1. Cation distribution and threshold displacement energy (TDE)

The unit cell of the spinel contains 56 atoms [8], with a generalized structural formula:



The structural stability of these materials under irradiation is a critical aspect; a key parameter for evaluating this stability is the TDE, defined as the minimum energy required to displace an atom from its position in the crystal lattice and create a

primary defect, such as a Frenkel pair. The TDE depends on multiple factors, including the crystal structure, the nature of chemical bonds, atomic mass, and crystallographic direction [9].

For the spinel structure of LMO, the cation distribution can be expressed as:

$$L_{\text{spinel}} = (\text{Li}^+)_{8a}[\text{Mn}^{3+/4+}]_{16d}(\text{O}^{2-})_{32e} \quad (1)$$

In LNMO:

$$L_{\text{LNMO}} = (\text{Li}^+)_{8a}[\text{Ni}_{16d}^{2+/3+}, \text{Mn}_{16d}^{3+/4+}](\text{O}^{2-})_{32e} \quad (2)$$

The TDE is related to crystal stability under radiation through models such as Kinchin–Pease and NRT (Norgett–Robinson–Torrens) [10]:

$$N_{d,\text{NRT}}(T_d) = \begin{cases} 0 & T_d < E_d \\ 1 & E_d < T_d < 2E_d \\ \eta \frac{T_d}{2E_d} & T_d > 2E_d \end{cases}, \quad (3)$$

where N_d is the number of displacements per atom, T_d is the deposited energy, E_d is the TDE, and η is the damage efficiency (~ 0.8) [11].

In the spinel structure, atoms in octahedral sites, such as Mn in LMO, generally exhibit a higher TDE than atoms in tetrahedral sites, such as Li, due to a greater number of bonds and higher local atomic density [12]. Covalent bonds, such as Ni–O in LNMO, are stronger than predominantly ionic bonds, such as Li–O in LMO, which also contributes to a higher TDE [13]. Furthermore, lighter atoms, such as Li, require less energy to be displaced than heavier atoms such as Mn or Ni [14]. It has been suggested that the presence of Jahn-Teller distortions, characteristic of Mn^{3+} in LMO, could weaken the lattice and contribute to a reduction in the TDE [15].

II.2. II.2 Effects of Ni doping

The substitution of Mn^{3+} by $\text{Ni}^{2+}/\text{Ni}^{3+}$ in LMO not only oxidizes part of the Mn to Mn^{4+} , but also appears to significantly reduce Jahn-Teller distortions, which potentially stabilizes the crystal structure and strengthens the Ni–O and Mn^{4+} –O bonds [16]. The substitution of Mn by Ni increases the effective local atomic density due to the higher atomic mass of nickel (58.7 vs. 54.9 u). This increased density contributes to a greater number of effective nearest neighbors and strengthens the local network, thereby raising the energy barriers for atomic displacement. The TDE of Ni atoms in LNMO is estimated to be between 70–120 eV, reflecting the strength of its covalent bonds with oxygen. These increases in TDE are directly proportional to the concentration of Ni, making LNMO more resistant to irradiation damage than LMO.

II.3. II.3 Atomic displacement cascades

When a target atom (the lattice atom) receives a recoil kinetic energy from an incident particle, becoming a Primary

Knock-on Atom (PKA), that exceeds its TDE, a displacement is initiated. This results in the atom being ejected from its lattice site. This displaced atom can collide with other neighboring atoms, transferring the remaining energy (in terms of kinetic energy) to other atoms. If this energy is sufficiently high, it can provoke an atomic displacement cascade that propagates through the crystal lattice, thus generating a large number of point defects such as vacancies and interstitials [17]. In the case of gamma irradiation, the maximum kinetic energy that a secondary electron can acquire is equal to the energy of the incident photon itself. The average energy transferred from such an electron to a PKA can be estimated by:

$$T = \frac{2E_e^2}{m_e c^2 + 2E_e}, \quad (4)$$

where E_e is the energy of the electron, m_e the rest mass of the electron and c the speed of light in vacuum. For relativistic approximations, though in practice for gamma interactions, Compton scattering dominates and the maximum electron recoil energy determines the potential for secondary ionization and, indirectly, atomic displacements. The gamma radiation considered in this work comes from a ^{60}Co source (1.17 and 1.33 MeV), consistent with the source available in our laboratory. These photon energies exceed typical TDE values, generating secondary electrons (Compton and photoelectric) that induce PKAs. The kinetic energy of these secondary electrons is used as input for the displacement cascade simulations.

III. III. MATERIALS AND METHODS

Given that the TDE for atoms within LMO and LNMO spinels have not been experimentally established, TDE values were inferred from those of atoms occupying similar lattice sites in compounds with analogous chemical bonding and crystal symmetry. In particular, experimental and computational studies on structurally related spinel oxides such as MgAl_2O_4 , LiFe_5O_8 , and NiCr_2O_4 were analyzed to infer trends in bond strength, coordination, and radiation response [18] [19] [20]. Based on this comparative research, an approximation for the TDE values in LMO (Table I) and LNMO (Table II) was proposed, guided by systematic trends in atomic mass, cation–oxygen bond covalency, and geometry site (tetrahedral vs. octahedral). First-principles calculations on analogous systems support that TDE ranges with local atomic density and bond strength, allowing reasonable extrapolation to LMO and LNMO [18] [19] [20].

Table 1. Ranges of displacement threshold energy for LiMn_2O_4

Atom	Z	E_d^{min} (eV)	E_d^{max} (eV)	E_d^{prom} (eV)
Li	3	10	100	20
Mn	25	40	100	70
O	8	40	70	55

Table 2. Ranges of displacement threshold energy for $\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4$

Atom	Z	$E_d^{\min}(\text{eV})$	$E_d^{\max}(\text{eV})$	$E_d^{\text{prom}}(\text{eV})$
Li	3	25	50	37.5
Ni	28	70	120	95
Mn	25	90	130	110
O	8	50	100	75

The phenomenon of atomic displacement cascades can be analyzed through the calculation of displacements per atom (dpa) cross-section, which quantifies the probability of total accumulated damage in the lattice. The cutoff energy values for the initiation of simple atomic displacement processes (E_c), related to the TDE, can be calculated using the equation;

$$E_c = \frac{2E_d}{1 - \alpha'} \quad (5)$$

where α is a factor depending on the mass of the involved atoms.

For the calculation of the dpa cross-section and E_c , the Monte Carlo assisted Classical Method (MCCM) program [21] was used, which employs classical theories of electron elastic scattering. The MCCM program uses only elastic electron scattering because elastic nuclear collisions transfer significant energy to atoms, while inelastic processes (ionization, etc.) produce secondary electrons with energies below the displacement threshold. Thus, inelastic contributions to atomic displacement are negligible, a standard approximation in computational radiation damage studies. The cutoff energies for the initiation of atomic displacement cascades (E_{cc}) were obtained by plotting the results from MCCM (dpa cross-section vs. kinetic energy) and determining the point at which the slope of the curve changes.

IV. IV. RESULTS AND DISCUSSION

Figures 1, 2, and 3 illustrate the calculation of dpa cross-section using the minimum, maximum, and average values of the TDE for each atom in LMO. The calculation of dpa cross-section using the minimum, maximum, and average values of the TDE for each atom in LNMO are shown in figures 4, 5 and 6.

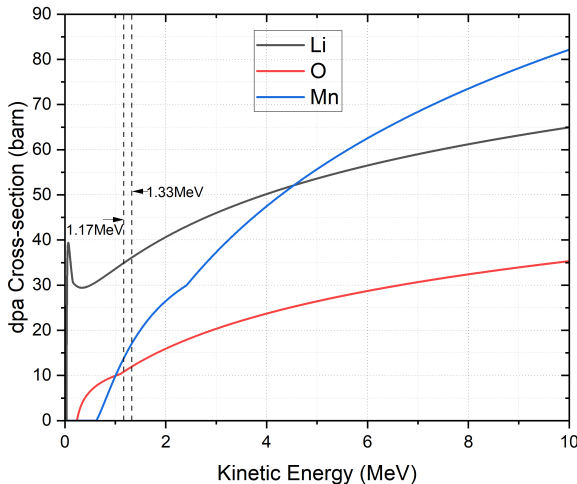


Figure 1. Relationship of dpa cross-section versus kinetic energy for the minimum TDE values of LMO.

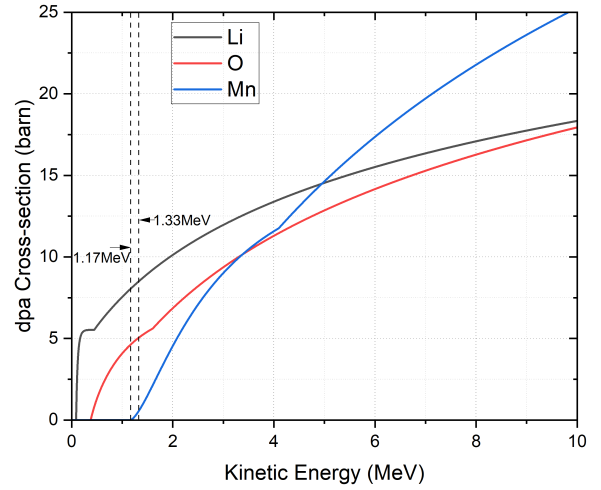


Figure 2. Relationship of dpa cross-section versus kinetic energy for the maximum TDE values of LMO.

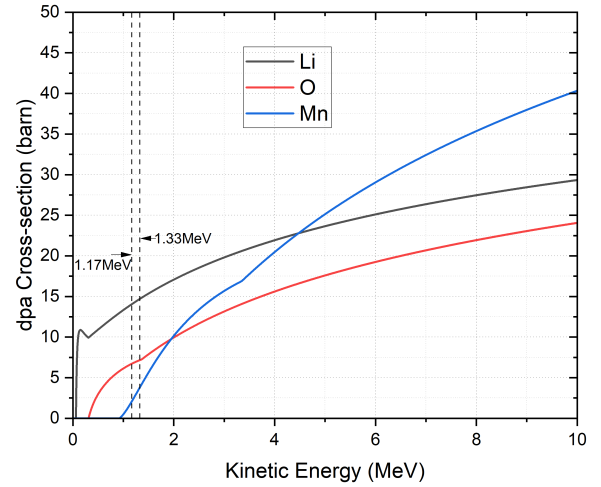


Figure 3. Relationship of dpa cross-section versus kinetic energy for the average TDE values of LMO.

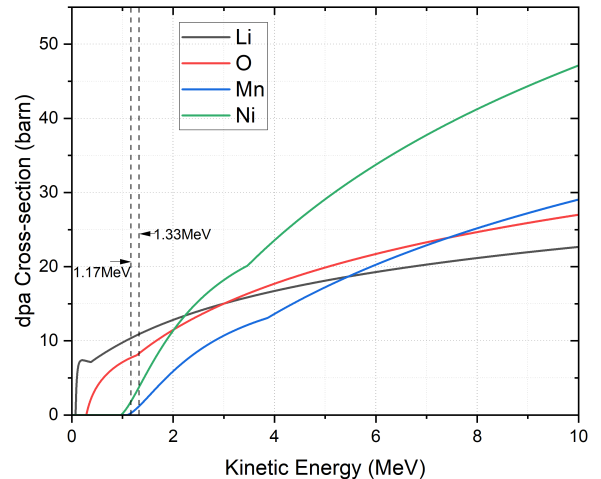


Figure 4. Relationship of dpa cross-section versus kinetic energy for the minimum TDE values of LNMO.

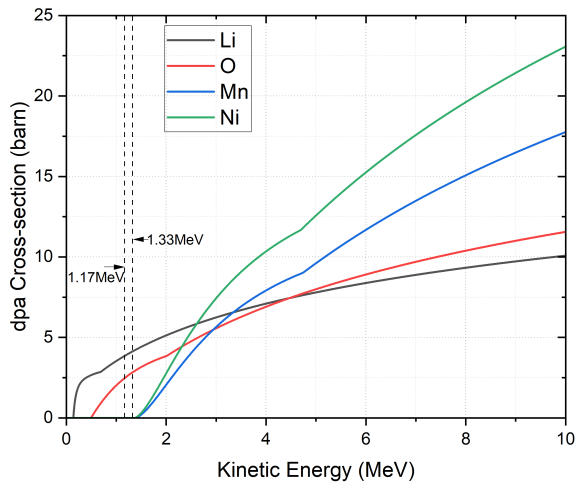


Figure 5. Relationship of dpa cross-section versus kinetic energy for the maximum TDE values of LNMO.

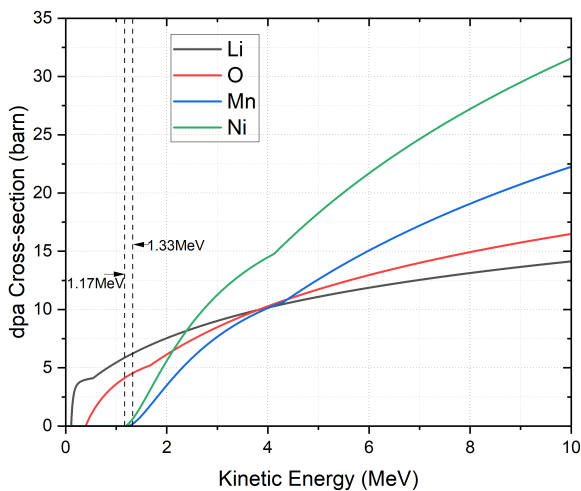


Figure 6. Relationship of dpa cross-section versus kinetic energy for the average TDE values of LNMO.

From the graphs, E_c and E_{cc} were extracted for each TDE value of atom in LMO (Table III) and LNMO (Table IV).

Table 3. Cutoff energy values for the initiation of simple atomic displacement processes and cutoff energies for the initiation of atomic displacement cascades, corresponding to each TDE value of each atom in LMO.

Atom	Z	E_d (eV)	E_c (MeV)	E_{ci} (MeV)
Li	3	10	0.031	0.157
		30	0.088	0.448
		20	0.060	0.308
Mn	25	40	0.626	2.411
		100	1.174	4.098
		70	0.926	3.347
O	8	40	0.238	1.096
		70	0.376	1.604
		55	0.310	1.365

Compared to Li, the Mn and Ni bonds require 2 to 3.6 times more displacement energy, reflecting their stabilizing role in the lattice. The probability of initiating a cascade is directly determined by the TDE; therefore, materials with high TDE, such as LNMO, have a higher threshold for cascade initiation, reducing the probability of forming cascades and thereby minimizing accumulated structural damage. Monte Carlo

simulations reveal that the dpa cross-sections for LNMO are systematically lower than those for LMO under equivalent irradiation conditions. This reduction is directly attributed to the higher TDE, which require greater energy to initiate damage processes. The relationship between TDE and damage accumulation follows trends predicted by theoretical models: materials with higher TDE accumulate fewer defects per unit of radiation dose, resulting in better stability of structural and electrochemical properties under prolonged irradiation.

Table 4. Cutoff energy values for the initiation of simple atomic displacement processes and cutoff energies for the initiation of atomic displacement cascades, corresponding to each TDE value of each atom in LNMO.

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V. CONCLUSIONS

This study indicates that the substitution of Mn by Ni in LNMO not only improves its electrochemical properties but also significantly increases its resistance to irradiation damage. Strengthening of Ni-O covalent bonds and oxidation of Mn^{3+} to Mn^{4+} may reduce Jahn-Teller distortions, which in turn could contribute to an elevation of the threshold displacement energy of the constituent atoms. The increase in TDE translates into a higher critical energy (E_c) and cascade initiation energy (E_{cc}), which decreases the probability of forming point defects and atomic cascades. The calculation of the dpa cross-section confirms that LNMO accumulates less structural damage for the same irradiation dose.

REFERENCES

- [1] G. B. Andreozzi and F. Princivalle, *Am. Mineral.* **87**, 838 (2002).
- [2] Y. Lin, F. Li, K. Zhao, S. Zou, X. Tan, Z. Shi, J. Fan, L. Ouyang, M. Zhu, and J. Liu, *Small Methods* **9**, 2402233 (2025).
- [3] H. Sun et al., *Adv. Funct. Mater.* **32**, 2112279 (2022).
- [4] L. Wan, Y. Deng, C. Yang, H. Xu, X. Qin, and G. Chen, *RSC Adv.* **12**, 30503 (2022).
- [5] M. M. Thackeray, P. J. Johnson, J. T. Vaughey, N. Li, and S. A. Hackney, *J. Mater. Chem.* **15**, 2257 (2005).
- [6] K. E. Sickafus et al., *Science* **289**, 748 (2000).
- [7] R. Arabolla et al., *Solid State Ionics* **324** (2018).
- [8] C. Biagioni and M. Pasero, *Am. Mineral.* **99**, 1254 (2014).
- [9] P. Dzerzanovsky and I. G. Barash, *Geol. Ore Deposits* **53**, 758 (2011).
- [10] I. M. Torrens and M. T. Robinson, *Phys. Rev. B* **9**, 5008 (1974).
- [11] M. J. Norgett, M. T. Robinson, and I. M. Torrens, *Nucl. Eng. Des.* **33**, 50 (1975).

- [12] R. Amin and I. Belharouk, *J. Power Sources* **348**, 311 (2017).
- [13] M. Kunduraci, J. F. Al-Sharab, and G. G. Amatucci, *Chem. Mater.* **18**, 3585 (2006).
- [14] J. H. Kim, N. P. W. Pieczonka, Z. Li, Y. Wu, S. Harris, and B. R. Powell, *Electrochim. Acta* **90**, 556 (2013).
- [15] L. Cai, Z. Liu, K. An, and C. Liang, *J. Mater. Chem. A* **1**, 6908 (2013).
- [16] A. J. A. Al-Hail et al., *ACS Appl. Energy Mater.* **3**, 6400 (2020).
- [17] M. T. Robinson and I. M. Torrens, *Phys. Rev. B* **9**, 5008 (1974).
- [18] W. A. Coghlan, F. W. Clinard, N. Itoh, and L. R. Greenwood, *J. Nucl. Mater.* **141–143**, 382 (1986).
- [19] S. Tan, W. Zhang, F. Jiao, Y. Zhou, L. Yang, W. Shi, and Z. Wang, *Cryst. Res. Technol.* **56**, 2100076 (2021).
- [20] L. Van Brutzel, P. Alvarez, and A. Chartier, *Nucl. Instrum. Methods Phys. Res. B* **326**, 278 (2014).
- [21] I. Piñera, C. M. Cruz, Y. Abreu, A. Leyva, A. E. Cabal, and P. Van Espen, in *2008 IEEE Nuclear Science Symposium Conference Record*, 2557 (2008).

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ADSORPTION OF PIPERAZINE-DITHIOCARBAMATE ON Au(111): AN ELECTROCHEMICAL SCANNING TUNNELING MICROSCOPY STUDY

ADSORCIÓN DE PIPERAZINA-DITIOCARBAMATO EN Au(111): ESTUDIO MEDIANTE MICROSCOPIA DE BARRIDO POR EFECTO TÚNEL ELECTROQUÍMICO

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* *In memoriam*

The adsorption process of piperazine-dithiocarbamate potassium salt, which occurs on the Au(111) surface, was studied by using electrochemical scanning tunneling microscopy. Perchloric acid and sodium hydroxide were used as electrolytes. The results revealed that, depending on the applied potential and the nature of the electrolyte, the entire molecule or just individual sulfur atoms were adsorbed forming different sulfur phases, instead of the entire molecule.

Mediante el empleo de la microscopía de barrido por efecto túnel en ambiente electroquímico, se estudió el proceso de adsorción de la sal ditiocarbamato-piperazina de potasio sobre la superficie de Au(111). Se emplearon ácido perclórico e hidróxido de sodio como electrolitos. Los resultados mostraron que, en dependencia del potencial aplicado y la naturaleza del electrolito, se produjo la adsorción de la molécula completa, o solamente de sus átomos de azufre, formando diferentes tipos de estructuras.

Keywords: Thin films, scanning tunneling microscopy, electrochemistry, microscopy of surfaces, interfaces.

I. INTRODUCTION

Dithiocarbamate is a sulfur-based functional group, and their compounds are employed as building blocks for self-assembled monolayers (SAMs) on gold surfaces. These SAMs can be easily prepared in liquid phase by deposition from solutions because of the high affinity between sulfur and gold atoms, with applications as electrochemical sensors and in the preparation of molecular devices [1–6]. Under certain conditions during the deposition process, only sulfur atoms are adsorbed on gold, by the breaking of the bond between sulfur and the rest of the molecule [7–11]. Under different conditions the entire molecule is adsorbed on the surface, thus forming SAMs [12, 13]. This behavior is strongly related to the chemical and physical properties of the dithiocarbamate solution (concentration, pH, temperature) [14–16].

Some aspects of the interaction between sulfur and gold have not been completely explained yet, like the adsorbate mobility [17], the ordering of atoms forming different structures or phases [18–21], the presence of vacancies or holes in the surface [21–23], the lifting of the surface reconstruction, the adsorption mechanism [17–25], and the surface sites where it takes place [21, 26–28]. By using electrochemical scanning tunneling microscopy (EC-STM) [29], the influence of the electrical potentials and pH in the processes of adsorption/desorption of the molecules or atoms on the surface can be studied in real time, together with the structure formation and surface modifications.

Dithiocarbamate adsorption has been previously studied by experimental techniques like X-ray photoelectron spectroscopy (XPS) [3, 6, 8], atomic force microscopy (AFM) and scanning tunneling microscopy (STM) [3, 7, 8, 11–13], but not by EC-STM. In this article, we used EC-STM for studying the behavior of the piperazine-dithiocarbamate of potassium molecules (K_2DTC_2pz) in solution, interacting with a polycrystalline Au(111) surface in acid (perchloric acid, $HClO_4$) and basic (sodium hydroxide, $NaOH$) environments.

II. EXPERIMENTAL

Starting materials: Potassium and sodium hydroxides (Alfa Aesar, p.a. quality); piperazine, perchloric acid, methanol, and carbon disulfide (Merck, p.a.). K_2DTC_2pz was synthesized as follows: 1 g of KOH was added to a solution containing 5 ML of methanol and 3 ML of CS_2 . This solution was stirred until the KOH was completely dissolved, and then 194.2 mg of piperazine were added. The resulting solution was reacted for 30–40 min, and afterwards, it was rotoevaporated until completely dried [7].

In situ STM images were taken at 298 K with a Digital Instruments Nanoscope E electrochemical scanning tunneling microscope (EC-STM) equipped with a bi-potentiostat, using tungsten tips, etched from a polycrystalline wire in aqueous NaOH. The tips were polymer coated to reduce the faradaic current at the tip-electrolyte interface. All images were recorded in the constant current mode, and processed with

the WSxM software [30].

The EC-STM electrochemical cell consists of an Au(111) polycrystalline thin film on a borosilicate substrate with an area of $12 \times 12 \text{ mm}^2$ (ArrandeeTM) as a working electrode (WE), two platinum wires served as counter and reference electrodes. The reported potentials (E) are in the saturated calomel electrode (SCE) scale ($E_{Pt} - E_{SCE} = 0.55 \text{ V}$) [31]. Before each experiment, the Au WE was annealed in a hydrogen flame for about 3 min and cooled down to room temperature. Samples were first immersed at open circuit potential (ocp) in aqueous 0.004 mM $\text{K}_2\text{DTC}_2\text{pz}$ in 0.5 M NaOH or HClO_4 . The samples were imaged in the most intense electro-reduction/oxidation peaks. Imaging potentials ranged from -1.4 to 0.5 V.

III. RESULTS AND DISCUSSION

Figure 1 shows the EC-STM images of an Au(111) surface immersed in the $\text{K}_2\text{DTC}_2\text{pz}$ solution in basic medium obtained at two different electrochemical potentials. At $E = -0.825 \text{ V}$ (Figure 1a), totally covered terraces by quasi-ordered structures were observed, composed of bright spots in rectangular-like arrays (region 1). At more positive potentials ($E = -0.790 \text{ V}$, Figure 1b), the coverage on the surface breaks with the order observed in Figure 1a. This image shows three different height features: small regions with several bright spots corresponding to atoms or arrays of atoms with different structures (region 2, 3, 4); a zone widely covered by a layer of adsorbate with no apparent order (5); and a few darker zones (6), corresponding to etch pits of the surface.

Figure 2a shows a closer inspection of region 1 of the modified gold surface, revealing more details of the rectangular-like arrangement, with well-ordered spots. This structure is formed by parallel chains of spots in either I and II directions, having intercalated bright and dark spots forming hexamer-like structures. The length of the chains is $(1.16 \pm 0.02) \text{ nm}$, the distance between the atoms in the chains is $(0.59 \pm 0.06) \text{ nm}$, and the separation between them is $(0.55 \pm 0.03) \text{ nm}$, as shown in profiles I and II (Figure 2 b and c). Taking into account that the heights in the profiles have an average value of $(0.16 \pm 0.03) \text{ nm}$, they might correspond to sulfur atoms from the molecule. This can be explained, considering that due to the presence of the gold surface, a strong interaction is established between the sulfur and gold atoms, yielding the adsorption of sulfur and breaking of sulfur-carbon bonds, leaving the rest of the dithiocarbamate molecule in the electrolyte solution.

Assuming a non-reconstructed Au(111) surface, this hexamer-like pattern can be described with a $\begin{pmatrix} 4 & 0 \\ 1 & \sqrt{3} \end{pmatrix}$ structure with an approximate coverage of 0.25 ML.

A zoom area of the squared region 2 from Figure 1b (Figure 3) presented several brilliant spots forming regular patterns composed of four atoms (tetramers). From the height profiles,

similar to those of the previous case, we concluded that these tetramers structures were composed only of sulfur atoms, with dimensions $(0.56 \pm 0.08) \times (0.63 \pm 0.08) \text{ nm}$. A comparison with the dimensions of the sulfur tetramers previously observed on Au(100) by STM ($0.57 \times 0.56 \text{ nm}$) [7] reveals that the tetramers observed under electrochemical conditions in the basic environment on this surface are smaller than the ones observed in air on Au(100). Assuming again that there was no Au(111) reconstruction, this phase can be

described with a $\begin{pmatrix} 2 & 0 \\ \sqrt{5}/2 & \sqrt{15}/2 \end{pmatrix}$ structure, that corresponds to a coverage of 0.2 ML. A zoom of region 3 in Figure 1b appears in Figure 4. This region also presents the sulfur atoms arranged in a quasi-rectangular array of dimensions $(1.54 \pm 0.08) \times (0.68 \pm 0.08) \text{ nm}$ in two orientations, being its structure $\begin{pmatrix} 9/2 & 3\sqrt{3}/2 \\ 5/2 & 5\sqrt{3}/4 \end{pmatrix}$, that corresponds to a very dilute coverage of 0.07 ML.

Region 4 also from Figure 1b was also magnified (Figure 5) to reveal very bright spots without any kind of order. The height of these spots is about $(0.28 \pm 0.03) \text{ nm}$, remarkably higher than the heights observed for the previously studied cases. We attributed these spots to the whole molecule anchored to the surface with a tilt of about 60° , which should explain why these points have a higher height.

The coexistence of several arrangements of sulfur atoms and the presence of $\text{K}_2\text{DTC}_2\text{pz}$ molecules in Figure 1b demonstrates that at this potential the system has a very dynamical behavior, being that all the sulfur atoms are not completely separated from the molecules, and not in their most stable arrangement on the Au surface, resulting in a coexistence of molecules and different arrangements of atoms.

In the case of perchloric acid as an electrolyte, at a potential $E = -0.447 \text{ V}$, an oblique-shaped array covering wide areas of the surface appears (Figure 6). From the profile, we can establish that the separation between the spots has a mean value of $(0.41 \pm 0.02) \times (0.35 \pm 0.05) \text{ nm}$, and the crystallographic angles have an average value of $(65 \pm 1)^\circ$ and $(115 \pm 2)^\circ$. This

structure can be mathematically described by a $\begin{pmatrix} \sqrt{2} & 0 \\ 3/5 & 3\sqrt{3}/5 \end{pmatrix}$ structure. The heights of the peaks in Figure 6, with an average value of $(0.25 \pm 0.03) \text{ nm}$, are similar than those present in Figure 5; therefore, this structure should be formed only by tilted molecules. Then, we can associate each bright spot with the $\text{K}_2\text{DTC}_2\text{pz}$ molecule, adsorbed over the Au(111) surface, forming a SAM with the afore mentioned structure, corresponding to a dense coverage of 0.75 ML.

Increasing E yields desorption of the sulfur atoms, disappearing the ordered structure, as was observed at $E = +103 \text{ mV}$ (Figure 7). The figure shows a diluted phase, where the spots corresponding to the sulfur atoms appear extended, indicating their mobility over the surface before desorption, which is completely reached at higher potentials.

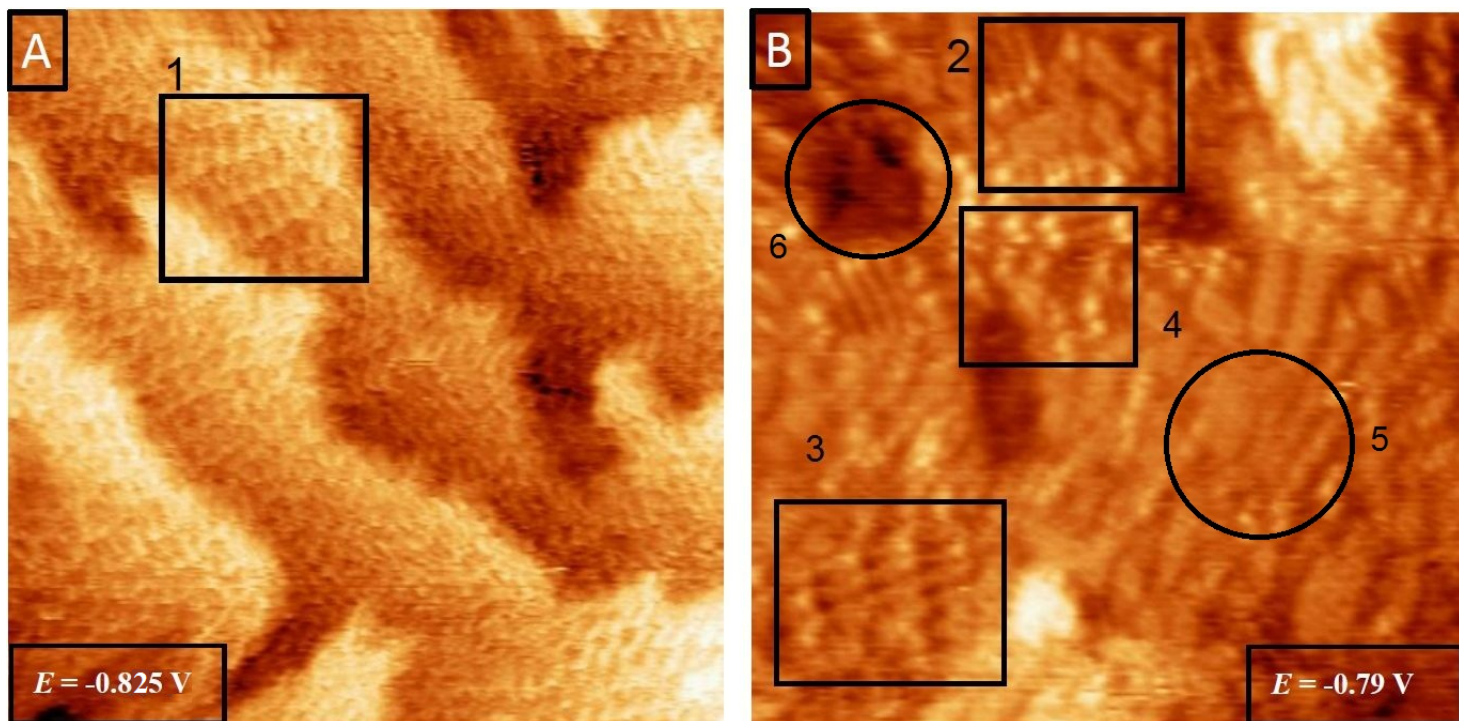


Figure 1. a) Unfiltered EC-STM image of $15.4 \times 15.5 \text{ nm}^2$ of the Au(111) surface modified with $\text{K}_2\text{DTC}_2\text{pz}$ in 0.5 M KOH: b) $E = -0.825 \text{ V}$, $V_{\text{bias}} = -64 \text{ mV}$, $I = 6 \text{ nA}$, $f = 5.8 \text{ Hz}$; c) $E = -0.790 \text{ V}$, $V_{\text{bias}} = -49 \text{ mV}$, $I = 5.4 \text{ nA}$, $f = 8.1 \text{ Hz}$.

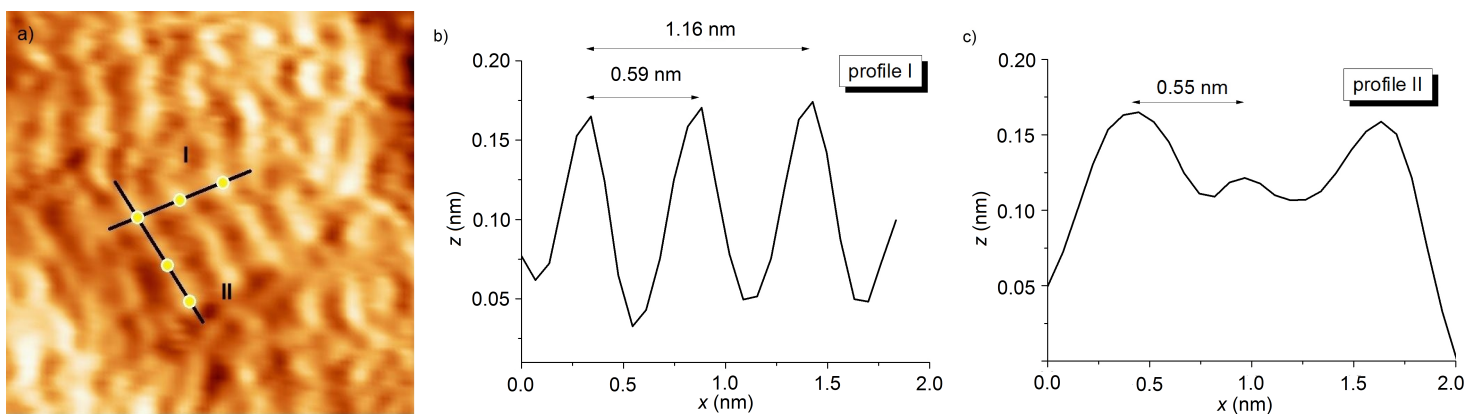


Figure 2. Unfiltered ECSTM image $4.7 \times 4.4 \text{ nm}^2$ from region inside box 1 on Figure 1a, showing rectangular patterns formed by six atoms. Line profiles I and II correspond to directions I and II (Figure 2b and c). Yellow circles mark the sulfur atoms.

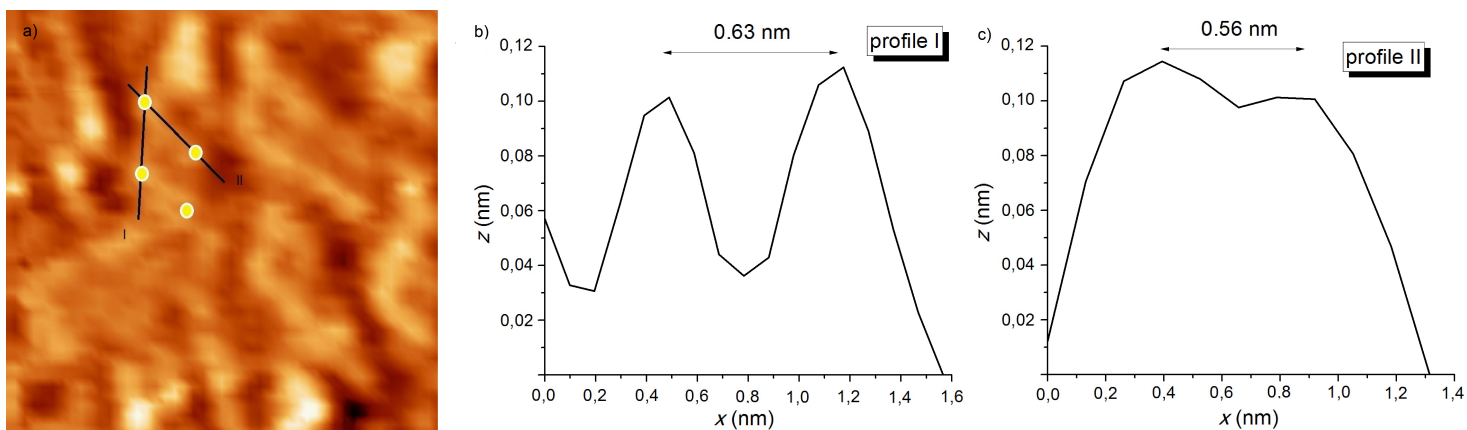


Figure 3. Unfiltered ECSTM image $4.7 \times 4.4 \text{ nm}^2$ from region inside box 2 on Figure 1b showing tetramers. Line profiles I and II correspond to directions I and II (Figure 3b and c). Yellow circles mark the sulfur atoms.

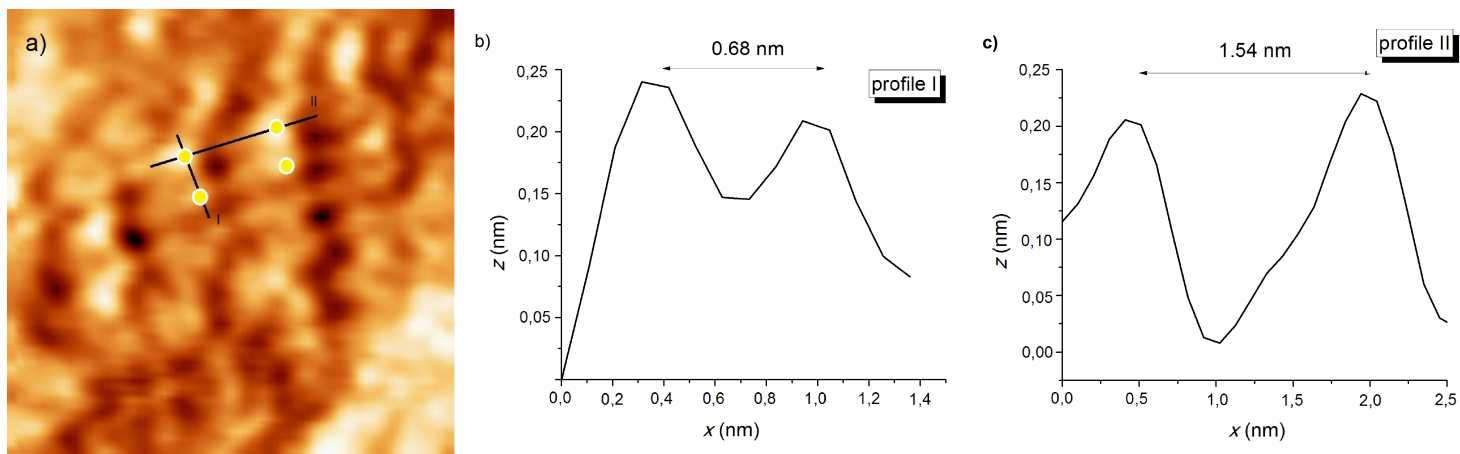


Figure 4. ECSTM image $7 \times 7 \text{ nm}^2$ from region inside box 3 on Figure 1b showing a quasi-rectangular array. Line profiles I and II correspond to directions I and II (Figure 4b and c). Yellow circles mark the sulfur atoms.

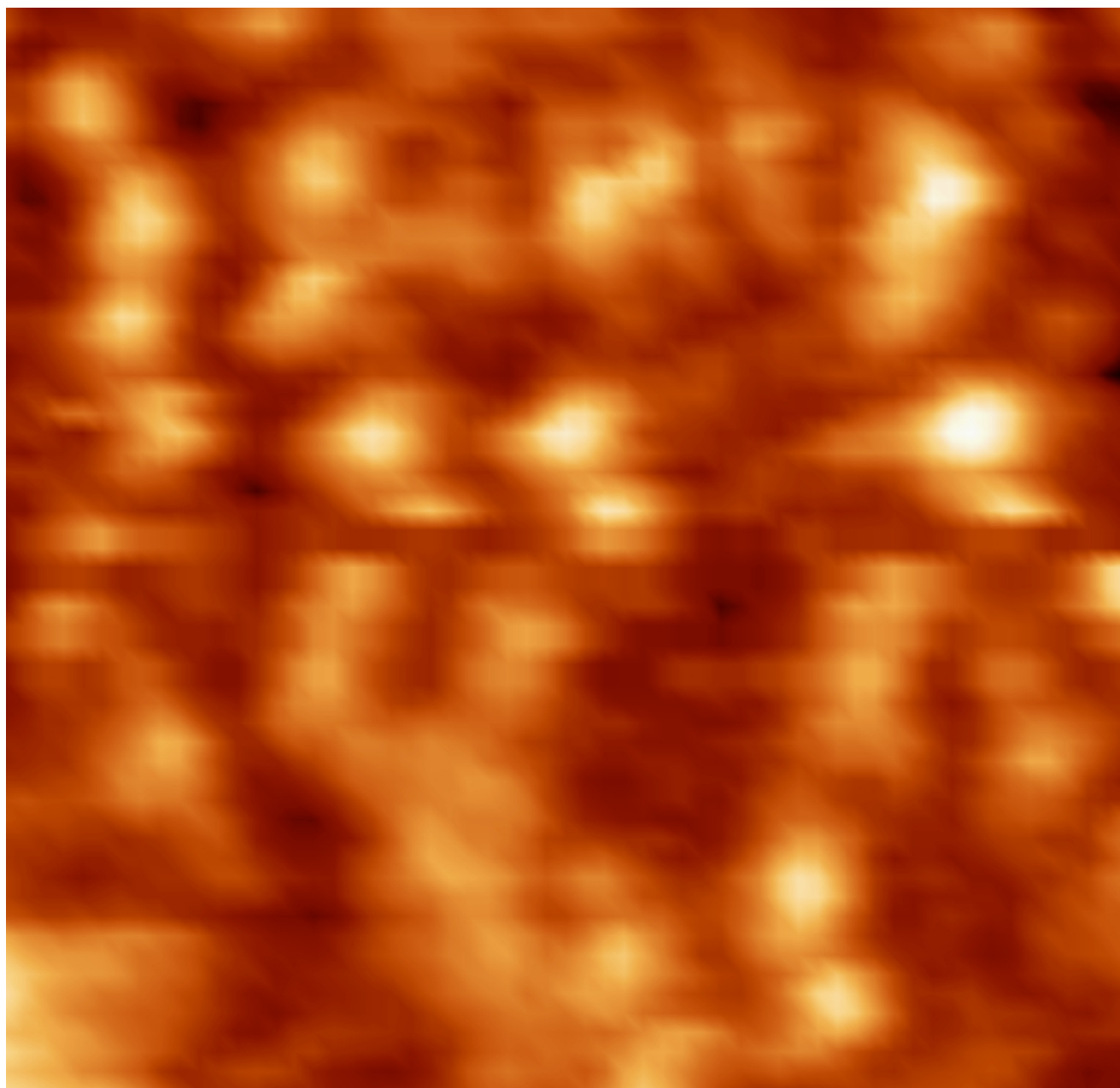


Figure 5. EC-STM image $6 \times 6 \text{ nm}^2$ of region 4 of Figure 1b showing very bright spots.

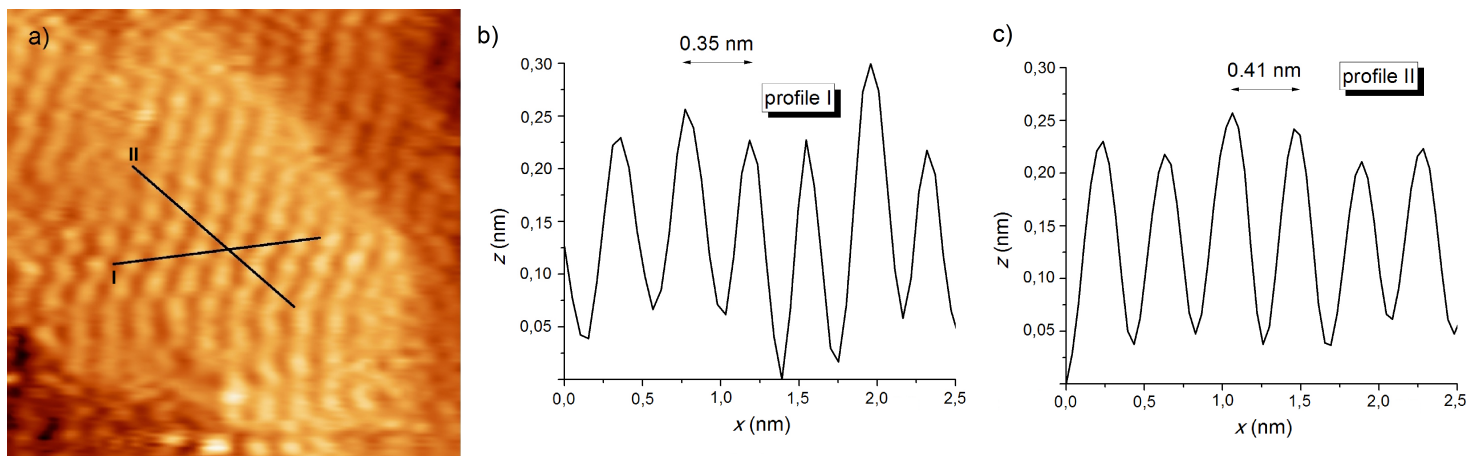


Figure 6. Unfiltered ECSTM image of $6 \times 6 \text{ nm}^2$ of the Au(111) modified with $\text{K}_2\text{DTC}_2\text{pz}$ in 0.5 M HClO_4 : a) $E = -0.447 \text{ V}$, $V_{\text{bias}} = -144 \text{ mV}$, $I = 24 \text{ nA}$, $f = 5.8 \text{ Hz}$. Line profiles I and II correspond to directions I and II (Figure 6b and c).

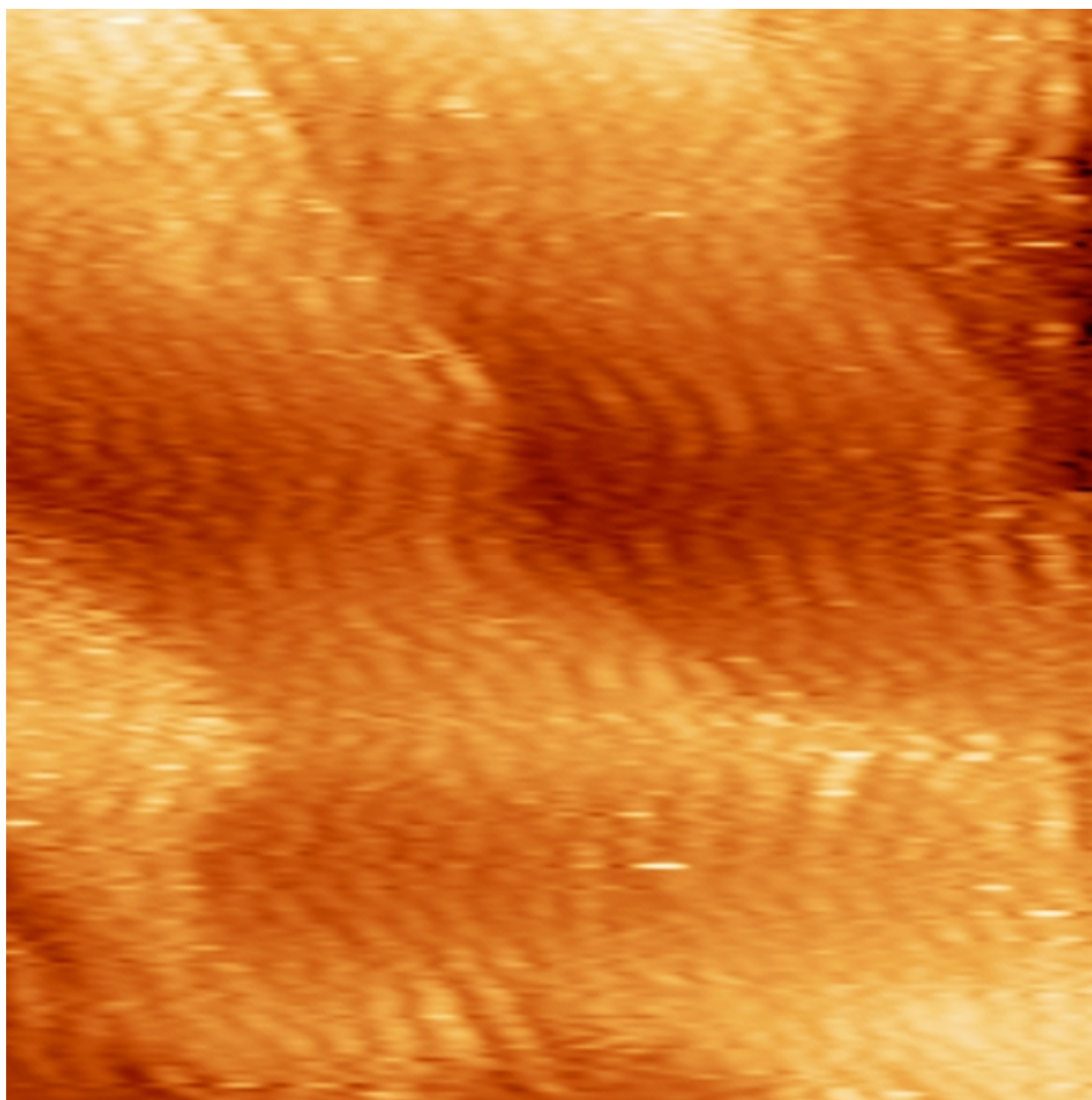


Figure 7. Unfiltered EC-STM image of $10 \times 10 \text{ nm}^2$ of the Au(111) modified with $\text{K}_2\text{DTC}_2\text{pz}$ in 0.5 M HClO_4 : a) $E = 103 \text{ mV}$, $V_{\text{bias}} = -144 \text{ mV}$, $I = 24 \text{ nA}$, $f = 3.9 \text{ Hz}$.

IV. CONCLUSIONS

The different structures formed by means of the adsorption of dithiocarbamates are studied by electrochemical scanning tunneling microscopy for the first time. These experiments were carried out taking into account the changes in the chemical environment (acid or basic) and the applied potential.

The presence of two different kinds of electrolytes brings us the opportunity to study the influence of chemical conditions on the adsorption of the piperazine-dithiocarbamate molecules. In both cases, depending on the potentials applied, we observed different features in the adsorbed layers: SAMs of sulfur atoms, more or less ordered, or without any ordered structures; and entire molecules of piperazine-dithiocarbamate. The resulting features are strongly dependent on the electrochemical environment and the applied potentials, dealing with the adsorption of the entire molecule or only sulfur atoms.

The presence, under certain conditions, of the entire molecule is remarkable because it allows us the possibility to study the electrochemical conditions to get the adsorption of individual sulfur atoms or the molecule, to resolve one of the most intriguing aspects of the dithiocarbamates adsorption: the conditions determining when the single sulfur atoms or the entire molecules are adsorbed.

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REFERENCES

- [1] W. E. Ford, D. Gao, F. Scholz, G. Nelles, F. von Wrochem, *Chem. Mater.*, **25**, 3603–3613 (2013).
- [2] W. E. Ford, D. Gao, F. Scholz, G. Nelles, F. von Wrochem, *ACS Nano*, **7**, 1943–1951 (2013).
- [3] D. Gao, F. Scholz, H.-G. Nothofer, W. Ford, U. Scherf, J. M. Wessels, A. Yasuda, F. von Wrochem, *J. Am. Chem. Soc.*, **133**, 5921–5930 (2011).
- [4] Z. Li, M. Smeu, T. H. Park, J. Rawson, Y. Xing, M. J. Therien, M. A. Ratner, E. Borguet, *Nano Lett.*, **14**, 5493–5499 (2014).
- [5] F. von Wrochem, D. Gao, H.-G. Nothofer, G. Nelles, J. M. Wessels, *Nat. Nanotechnol.*, **5**, 618–624 (2010).
- [6] D. Meyer, T. Schäfer, P. Schulz, S. Jung, J. Rittich, D. Mokros, I. Segger, F. Maercks, C. Effertz, R. Mazzarello, M. Wuttig, *Langmuir*, **32**, 8812–8817 (2016).
- [7] J. A. Martínez, J. Valenzuela B., R. Cao Milán, J. Herrera, M. H. Farías, M. P. Hernández, *Appl. Surf. Sci.*, **320**, 287–293 (2014).
- [8] J. A. Martínez, J. Valenzuela, C. E. Hernández-Tamargo, R. Cao-Milán, J. A. Herrera, J. A. Díaz, M. H. Farías, H. Mikosch, M. P. Hernández, *Appl. Surf. Sci.*, **345**, 394–399 (2015).
- [9] C. E. Hernández-Tamargo, R. Barzaga, H. Mikosch, J. A. Martínez, J. A. Herrera, M. H. Farías, M. P. Hernández, *Phys. Chem. Chem. Phys.*, **18**, 29987–29998 (2016).
- [10] C. E. Hernández-Tamargo, A. L. Montero-Alejo, D. Codorníu Pujals, H. Mikosch, M. P. Hernández, *J. Chem. Phys.*, **141**, 044713-1–10 (2014).
- [11] R. Barzaga, J. A. Martínez, M. H. Farías, M. P. Hernández, *J. Phys. Chem. C*, **123**, 12183–12194 (2019).
- [12] A. F. Raigoza, G. Kolettis, D. A. Villalba, S. A. Kandel, *J. Phys. Chem. C*, **115**, 20274–20281 (2011).
- [13] P. Morf, N. Ballav, M. Putero, F. von Wrochem, J. M. Wessels, T. A. Jung, *J. Phys. Chem. Lett.*, **1**, 813–816 (2010).
- [14] J. C. Love, L. A. Estroff, J. K. Kriebel, R. G. Nuzzo, G. M. Whitesides, *Chem. Rev.*, **105**, 1103–1169 (2005).
- [15] R. G. Nuzzo, D. L. Allara, *J. Am. Chem. Soc.*, **105**, 4481–4483 (1983).
- [16] A. H. A. Mamun, J. R. Hahn, *Surf. Sci.*, **606**, 664–669 (2012).
- [17] K. M. Koczkur, E. M. Hamed, A. Houmam, *Langmuir*, **27**, 12270–12274 (2011).
- [18] A. Houmam, K. M. Koczkur, G. Moula, E. M. Hamed, *ChemPhysChem*, **13**, 1240–1245 (2012).
- [19] A. Houmam, H. Muhammad, K. M. Koczkur, *Langmuir*, **28**, 16881–16889 (2012).
- [20] C. Schlaup, D. Friebe, P. Broekmann, K. Wandelt, *Surf. Sci.*, **602**, 864–870 (2008).
- [21] C. Vericat, M. E. Vela, J. Gago, R. C. Salvarezza, *Electrochim. Acta*, **49**, 3643–3649 (2004).
- [22] M. M. Biener, J. Biener, C. M. Friend, *Langmuir*, **21**, 1668 (2005).
- [23] M. Biener, J. Biener, C. M. Friend, *Surf. Sci.*, **601**, 1659–1667 (2007).
- [24] M. E. Vela, H. Martin, C. Vericat, G. Andreasen, A. Hernández Creus, R. C. Salvarezza, *J. Phys. Chem. B*, **104**, 11878–11882 (2000).
- [25] H. Walen, D.-J. Liu, J. Oh, H. J. Yang, Y. Kim, P. A. Thiel, *J. Phys. Chem. C*, **119**, 21000–21017 (2015).
- [26] P. G. Lustemberg, C. Vericat, G. A. Benítez, M. E. Vela, N. Tognalli, A. Fainstein, M. L. Martiarena, R. C. Salvarezza, *J. Phys. Chem. C*, **112**, 11394–11402 (2008).
- [27] S. Y. Quek, M. M. Biener, J. Biener, J. Bhattacharjee, C. M. Friend, U. V. Waghmare, E. Kaxiras, *J. Phys. Chem. B*, **110**, 15663–15665 (2006).
- [28] C. Vericat, G. Andreasen, M. E. Vela, R. C. Salvarezza, *J. Phys. Chem. B*, **104**, 302–307 (2000).
- [29] R. Wiesendanger, *Scanning Probe Microscopy and Spectroscopy*, Cambridge University Press, 1994, pp. 283–284.
- [30] I. Horcas, R. Fernández, J. M. Gómez-Rodríguez, J. Colchero, J. Gómez-Herrero, A. M. Baró, *Rev. Sci. Instrum.*, **78**, 013705 (2007).
- [31] A. Cuesta, M. Kleinert, D. M. Kolb, *Phys. Chem. Chem. Phys.*, **2**, 5684–5690 (2000).

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TEMPERATURE-DEPENDENT RESISTIVITY AND CONDUCTION MECHANISMS IN Co AND F CODOPED NiO THIN FILMS

RESISTIVIDAD Y MECANISMOS DE CONDUCCIÓN DEPENDIENTES DE LA TEMPERATURA EN CAPAS DELGADAS DE NiO CODOPADOS CON Co Y F

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Co- and F-codoped NiO thin films were successfully deposited on glass substrates using the pneumatic spray deposition method at 420 °C. The influence of temperature (T) and dopant concentrations on the electrical and optical properties were investigated. Electrical measurements were carried out in two stages by evaluating the voltage and current over the temperature range of 30–180 °C. The temperature affected both voltage and current, with higher T's leading to an enhanced electrical response. The lowest electrical resistivity was achieved for the film doped with 2% Co and 12% F. Optical analysis revealed that the films exhibited high transparency in the visible region. Furthermore, the optical band gap increased with increasing Co and F concentrations in all samples. A minimum Urbach energy of 0.342 eV was observed for the film containing 2% Co and 8% F, indicating a reduction in localized states within the band tails and an improvement in optical quality.

Se depositaron exitosamente películas delgadas de NiO codopadas con Co y F sobre sustratos de vidrio utilizando el método de deposición por aspersión neumática a 420 °C. Se investigó la influencia de la temperatura (T) y las concentraciones de dopantes en las propiedades eléctricas y ópticas. Las mediciones eléctricas se realizaron en dos etapas, evaluando el voltaje y la corriente en el rango de temperatura de 30–180 °C. La temperatura afectó tanto al voltaje como a la corriente, observándose que temperaturas más altas conducen a una respuesta eléctrica mejorada. La resistividad eléctrica más baja se obtuvo para la película dopada con 2% de Co y 12% de F. El análisis óptico reveló que las películas exhibieron una alta transparencia en la región visible. Además, el gap de energía óptica aumentó con el incremento de las concentraciones de Co y F en todas las muestras. Se observó una energía de Urbach mínima de 0.342 eV para la película que contenía 2% de Co y 8% de F, lo que indica una reducción en los estados localizados dentro de las colas de banda y una mejora en la calidad óptica.

Keywords: NiO; Thin films (láminas delgadas); Co and F cooping (codopaje con Co y F); TCO; spray pneumatic method (Método del Spray Neumático)

I. INTRODUCTION

Nickel oxide (NiO) is considered an important semiconductor for environmental monitoring due to its ability to detect hazardous gases [1]. It has been employed in a wide range of applications, including gas sensors, fuel-cell electrodes, thermoelectric systems, dye-sensitized solar cells (DSSCs), electrochromic display materials, and catalytic processes [2–8]. For gas-sensing applications, the selection of a suitable material depends on understanding its interaction mechanisms, which are strongly related to its semiconducting electrical behavior and optical transparency. Experimental studies have demonstrated that NiO possesses high optical transparency along with acceptable electrical conductivity under various preparation conditions. Moreover, NiO thin films exhibit a direct optical band gap typically ranging from 3.5 to 4.3 eV [9,10].

The main objective of this work is to investigate a new material consisting of Co- and F-codoped NiO thin films intended for use as p-type transparent conducting oxides. Regarding the choice of Co and F co-dopants, cobalt (Co) was selected as a transition metal dopant due to its ability to substitute Ni²⁺ sites in NiO and introduce additional 3d

states, which can significantly modify the electronic structure, defect density, and magnetic/electrical properties. Fluorine (F), on the other hand, was chosen as an anion dopant because it can replace oxygen (O²⁻) sites and act as an effective shallow donor, thereby increasing carrier concentration and improving electrical conductivity. The combined Co and F co-doping strategy was therefore employed to simultaneously tune both cationic and anionic sublattices, aiming to achieve a synergistic improvement in structural, optical, and electrical properties. To the best of our knowledge, NiO thin films simultaneously doped with Co and F have not been previously reported. The advantages of this co-doping approach include enhanced control over defect states, improved tunability of band structure, and simultaneous modulation of conductivity and optical transparency. Previous studies on codoped NiO have mainly focused on other combinations, such as Fe–Li, Li–Cu, and Li–Ti systems.

The selected doping concentrations were maintained within a low levels to prevent secondary phase formation and ensure that the dopants remained below the solubility limit of the NiO lattice [11]. This approach enables the investigation of defect engineering and lattice perturbation effects while minimizing the influence of structural phase transitions [12,13]. Egbo

et al. [14] reported that effective p-type doping in NiO requires dopants with low formation and ionization energies to enhance solubility and carrier concentration. However, excessive doping can induce compensating donor defects, reducing doping efficiency and p-type conductivity.

Yan et al. [15] investigated the structural and magnetic properties of $\text{Ni}_{0.98}\text{Fe}_{0.02}\text{O}$ and $\text{Ni}_{0.93}\text{Fe}_{0.02}\text{Li}_{0.05}\text{O}$ thin films prepared by pulsed laser deposition. The samples exhibited ferromagnetic behavior at room temperature, and Li codoping was found to significantly enhance the saturation magnetization of $\text{Ni}_{0.98}\text{Fe}_{0.02}\text{O}$. The authors suggested that the dopants occupy substitutional lattice sites. When Li ions are incorporated into NiO, strong hybridization occurs at the Fermi level between the spin-split acceptor band and the Fe 3d electronic states.

Chen et al. [16] prepared p-type Li-Cu codoped NiO thin films using a chemical solution deposition method and evaluated their optical and electrical performance. The results showed that, for $\text{Li}_x\text{Cu}_{0.1}\text{Ni}_{0.9-x}\text{O}$ compositions, both optical transmittance and electrical conductivity increased with higher Li concentration (x). In addition, the resistivity of the deposited films decreased significantly, reaching $0.046 \Omega \cdot \text{cm}$ for the $\text{Li}_x\text{Cu}_{0.1}\text{Ni}_{0.8}\text{O}$ thin film.

Qureshi et al. [17] explored Li- and Ti-codoped NiO nanocomposites for gas-sensing applications at room temperature. Transmission electron microscopy (TEM) analysis revealed particle sizes in the range of 5–40 nm. The sensor exhibited its highest sensitivity toward toluene vapor under room-temperature operating conditions.

In this study, Co- and F-codoped NiO thin films were synthesized using a pneumatic spray deposition technique at 420°C . The optical and electrical properties were analyzed as a function of dopant concentration, and the electrical behavior was further evaluated over a temperature range of $30\text{--}180^\circ\text{C}$.

II. EXPERIMENTAL PROCEDURE

For the preparation of Co- and F-codoped NiO films, precursor solutions were obtained by dissolving 0.1 mol.l⁻¹ nickel chloride hexahydrate ($\text{NiCl}_2 \cdot 6\text{H}_2\text{O}$, CAS 7791-20-0) (99.7 % purity) together with cobalt chloride dihydrate ($\text{CoCl}_2 \cdot 2\text{H}_2\text{O}$, CAS 14216-74-1) (99.8 % purity), using Co/Ni ratios of 0.02 and 0.03. Ammonium fluoride (NH_4F , CAS 12125-01-8) (98 % purity) was added as the fluorine source at F/Ni ratios of 0.04, 0.08, and 0.12. The reagents were dissolved in equal volumes of absolute ethanol (99.995 % purity). Three drops of HCl were introduced as a stabilizing agent, and the resulting mixture was stirred for 120 minutes at 50°C until a clear, transparent solution was obtained.

The five samples of Co- and F codoped NiO precursor solutions were deposited onto heated glass substrates using the pneumatic spray technique. The solution was atomized into fine droplets with an average diameter of approximately $25 \mu\text{m}$. Deposition was carried out at a substrate temperature of 420°C and a solution flow rate of $2 \text{ ml} \cdot \text{min}^{-1}$, resulting in uniform thin film formation.

The optical transmittance of the deposited films was measured in the $300 - 700 \text{ nm}$ wavelength range using a UV-visible spectrophotometer (LAMBDA 25). The electrical resistance and resistivity of the films were determined using the four-point probe technique with a Keithley 2611B SourceMeter SMU. This instrument provides high-precision current measurements with excellent sensitivity in the picoampere (pA) to nanoampere (nA) range, enabling accurate characterization of highly resistive thin films.

The stabilization periods were applied during the temperature-dependent electrical conductivity measurements, and reproducibility was carefully verified during both heating and cooling cycles. Before each measurement point, the sample was allowed to reach thermal equilibrium at the target temperature. A stabilization time of approximately 2–5 minutes was used after each temperature change to ensure stable temperature and electrical signal. This minimized transient effects and ensured reliable conductivity values. Measurements were then repeated over complete heating and cooling cycles under identical conditions. The resulting conductivity curves showed good agreement between both cycles, with negligible thermal lag, confirming the stability, accuracy, and reproducibility of the measurements. The experimental setup was maintained under controlled laboratory conditions, with precautions taken to minimize electromagnetic interference, mechanical vibrations, and environmental disturbances.

III. RESULTS AND DISCUSSION

III.1. Electrical resistivity Co and F codoped NiO thin films

The electrical properties of Co- and F-codoped NiO thin films were investigated using the four-point probe method over a temperature range of $30\text{--}180^\circ\text{C}$. Measurements were conducted in two stages: in the first stage, the voltage and current of the films were recorded as the temperature increased from 30 to 180°C ; in the second stage, the same parameters were measured while the temperature decreased from 180 to 30°C . In order to study the effect of Co and F codoping on the electrical properties of NiO thin films, we made electrical measurements (sheet resistance R_{sh} , resistivity ρ and conductivity σ) as a function of Co and F concentrations. The sheet resistance of the films was calculated using the following relation [18]:

$$R_{sh} = \frac{\pi}{\ln 2} \cdot \frac{V}{I} \quad (1)$$

Here, (I) represents the measured current and (V) the measured voltage. Regarding the conversion from electrical measurements (mV and nA range) to resistivity values ($\Omega \cdot \text{cm}$), the calculation of resistivity and conductivity was performed using the following relations [19]:

$$\rho = dR_{sh} \quad (2)$$

$$\rho = \frac{1}{\sigma} \quad (3)$$

where ρ is the resistivity, d is the film thickness, R_{sh} is the sheet resistance, and σ is the conductivity.

Figure 1. Temperature dependence of voltage and electrical conductivity during heating and cooling cycles for Co and F codoped NiO thin films.

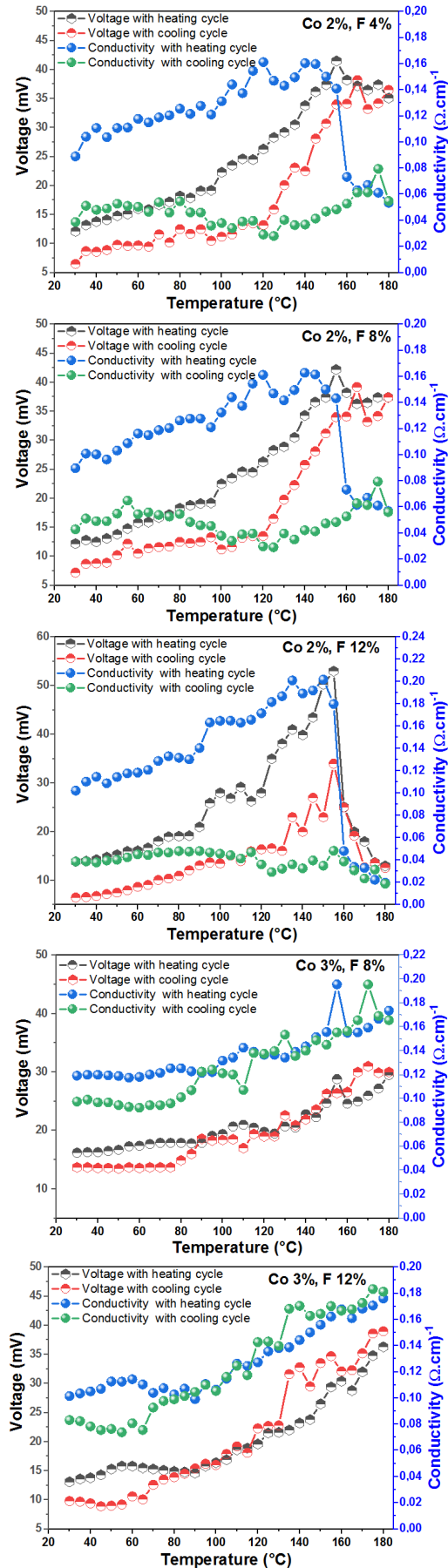


Figure 1 illustrates the variation of voltage with temperature for the Co- and F-codoped NiO films. It can be observed that the voltage increases with increasing temperature during the heating cycle (30 – 180 °C) and decreases with decreasing temperature during the cooling cycle (180 – 30 °C). Moreover, the voltage values measured during the heating cycle were consistently higher than those measured during the cooling cycle. This behavior is likely due to a reduction in the number of mobile charge carriers upon cooling, these results indicate that all deposited Co- and F-codoped NiO thin films are p-type semiconductors [20,21]. The optimum voltage was observed at approximately 160 °C for all deposited films, with the highest value recorded for the film co-doped with 2 % Co and 12 % F.

The electrical conductivity exhibited a different trend during the heating cycle. It initially increased with increasing temperature from 30 to 160 °C, reaching a maximum value at approximately 150–160 °C. This behavior confirms the semiconducting nature of the codoped NiO films [20], as the supplied thermal energy promotes charge-carrier excitation, thereby enhancing electrical conduction [22, 23]. However, further increasing the temperature beyond this range led to a significant reduction in the conductivity of certain samples. This behavior may be associated with structural rearrangements, increased carrier scattering, desorption of surface species, or the activation of defect states that reduce the concentration of free carriers [20–23].

During the cooling cycle, both voltage and conductivity followed different paths compared to those observed during heating cycle, resulting in a noticeable hysteresis effect. Mohiuddin and Hoa [24] reported that the electrical conductivity exhibits different behaviors during the heating and cooling cycles, leading to the occurrence of electrical hysteresis.

The voltage remained relatively high during cooling before gradually decreasing, while the conductivity did not fully recover its initial values measured during the heating cycle. Such hysteresis behavior is commonly observed in metal oxide semiconductors and may originate from irreversible or slowly reversible processes, including defect redistribution, oxygen adsorption/ desorption, charge-carrier trapping and detrapping of charge carriers, or thermally induced modifications in grain boundary potentials [20–23, 25].

Figure 2 shows the variation of voltage as a function of the measured current for for Co and F codoped NiO thin films, representing their current–voltage (I–V) characteristics. All samples show an increase in voltage with increasing measured current; however, some films exhibits nonlinear I–V behavior and a pronounced hysteresis effect, indicating differences in charge transport mechanisms between the heating and cooling processes, these results indicate that all deposited Co- and F-codoped NiO thin films are p-type semiconductors [26, 27]. The NiO thin film codoped with 2 % Co and 12 % F exhibited improved absorber-layer quality and enhanced

open-circuit voltage, reaching a maximum value of 53 mV at 155 °C.

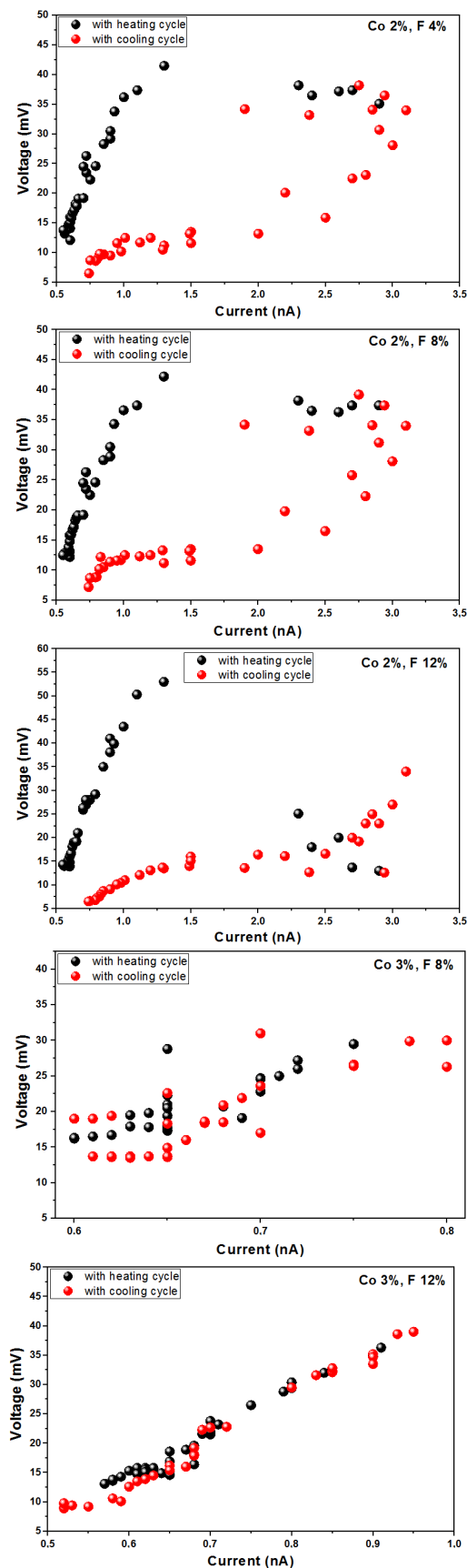


Figure 2. Current–voltage (I–V) characteristics of the Co- and F-codoped NiO thin films measured during the heating and cooling cycles.

Different current ranges were used in Figure 2 to obtain accurate I–V characteristics for each sample, as resistance varies with composition. Co and F codoping changes carrier concentration, defect density, and conductivity of NiO films. Thus, some samples show high resistance and low current, while others exhibit higher conductivity [28]. A single fixed range would reduce resolution or cause saturation. Therefore, the measurement range was adjusted for each sample to keep signals within the instrument’s optimal sensitivity, ensuring reliable and precise results.

Figure 3 shows the variation of electrical conductivity of Co and F codoped NiO thin films as a function of (a) heating cycle (b) cooling cycle. During the heating cycle (Figure 3a), all samples show a decrease in electrical resistivity with increasing temperature, indicating a negative temperature coefficient of resistance characteristic of semiconducting behavior. Similar observations have been reported in the literature [29, 30]. The observed behavior is indicative of thermally activated charge transport, whereby elevated temperatures promote charge-carrier mobility and increase the concentration of thermally excited carriers. Significant variations in resistivity are evident among the investigated compositions. Notably, the 2% Co–12% F co-doped films exhibit the lowest resistivity values, suggesting that increased co-doping concentrations enhance electrical conduction. This improvement can be associated with the generation of additional electrically active defects (e.g., oxygen vacancies) and enhanced carrier activation, both of which contribute to an increase in free-carrier density and charge-transport efficiency.

During the cooling cycle (Figure 3b), the resistivity does not fully return to its initial values. Indeed, the cooling resistivity is higher than the heating resistivity, resulting in a pronounced thermal hysteresis between the heating and cooling curves. Similar observations have been reported in the literature [20, 21, 31]. This behavior suggests the occurrence of irreversible or partially reversible changes during thermal cycling, such as defect reconfiguration, charge-carrier trapping/ detrapping, or the formation of metastable states. The incorporation of Co and F dopants may contribute to these effects by modifying the defect structure and carrier dynamics.

The increase in resistivity during cooling indicates a reduction in the concentration or mobility of thermally activated holes, which are the majority charge carriers in p-type NiO [20, 21], further emphasizing the influence of defect-related mechanisms on the electrical behavior of the films.

The decrease in resistivity with increasing temperature confirms the semiconducting behavior of the Co- and F-codoped NiO films. This behavior is associated with the thermal activation of holes, which are the majority charge carriers in p-type NiO and originate mainly from nickel vacancies and related acceptor defects. Similar observations have been reported in the literature [20–24]. However, the results confirm that Co–F co-doping strongly influences the electrical transport properties of NiO thin films, and the observed hysteresis highlights the role of defect chemistry and thermal activation processes in controlling conductivity.

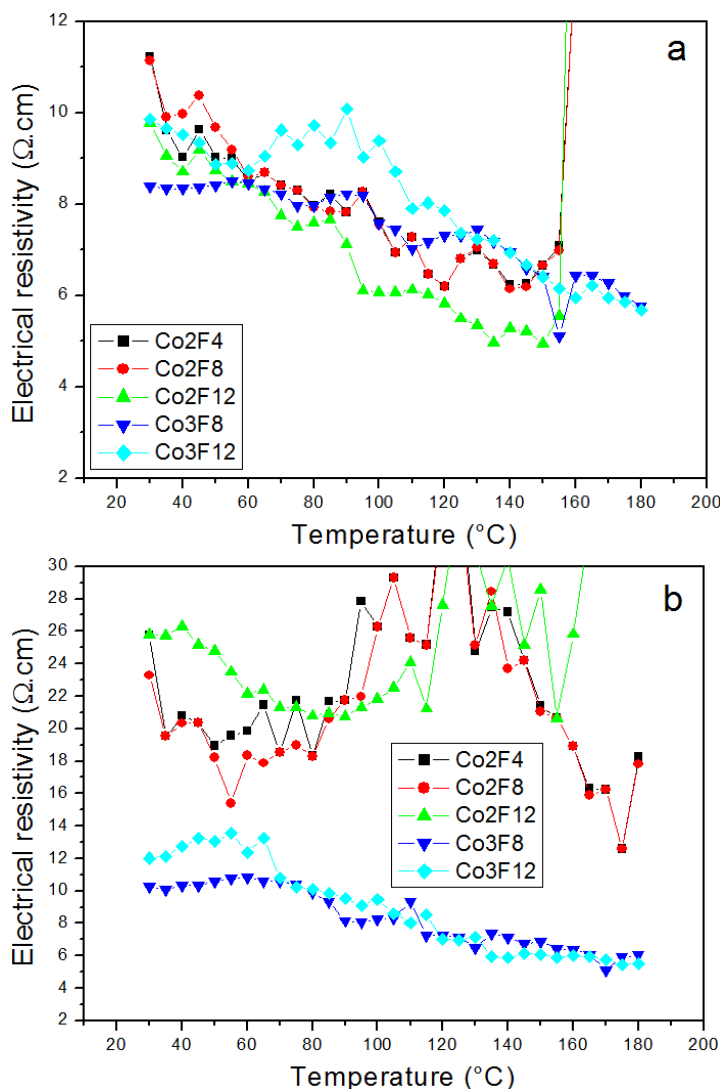


Figure 3. Variation of electrical conductivity of Co and F codoped NiO thin films as a function of (a): heating cycle (b): cooling cycle.

III.2. Optical property of Co and F codoped NiO thin films

The optical transmittance spectra of Co- and F-codoped NiO thin films at various dopant concentrations are shown in Figure 4, measured over the wavelength range of 300–700 nm. The films exhibited their highest transmittance in the visible region, ranging from 30 % to 65 %. Notably, the film codoped with 3 % Co and 12 % F demonstrated superior transparency, which can be attributed to the substitutional incorporation of Co into the Ni lattice [32]. Furthermore, the enhanced transparency of this film is also associated with the higher F doping concentration, highlighting the combined effect of Co and F codoping on optical performance.

Figure 5 illustrates the absorbance spectra of Co and F codoped NiO thin films in the wavelength range of 300–700 nm. All samples exhibit strong absorption in the UV region followed by a gradual decrease toward the visible region. The film containing 2 % Co and 4 % F shows the highest absorbance, while increasing the fluorine concentration

results in a progressive reduction in absorbance. A similar trend is observed for films doped with 3 % Co, with the 3 % Co–12 % F sample exhibiting the lowest absorbance. This behavior suggests that increasing Co and F concentrations enhances the optical transparency of the films and may be associated with modifications in the electronic structure and defect density of the NiO matrix [30,31].

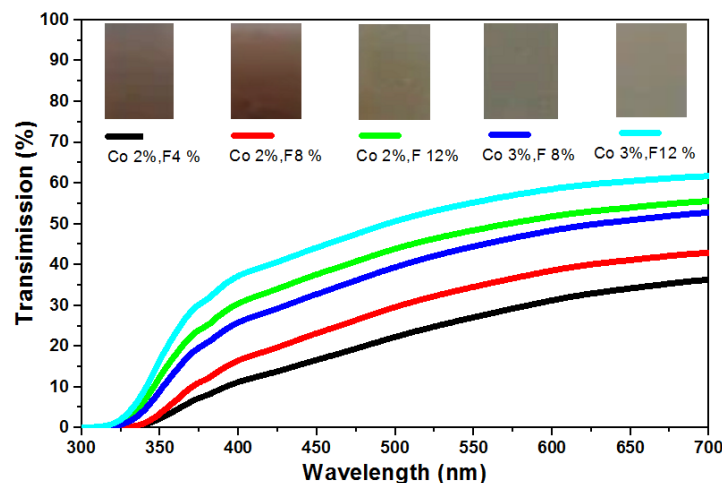


Figure 4. Transmission spectra of Co and F codoped NiO thin films as a function of Co and F concentrations.

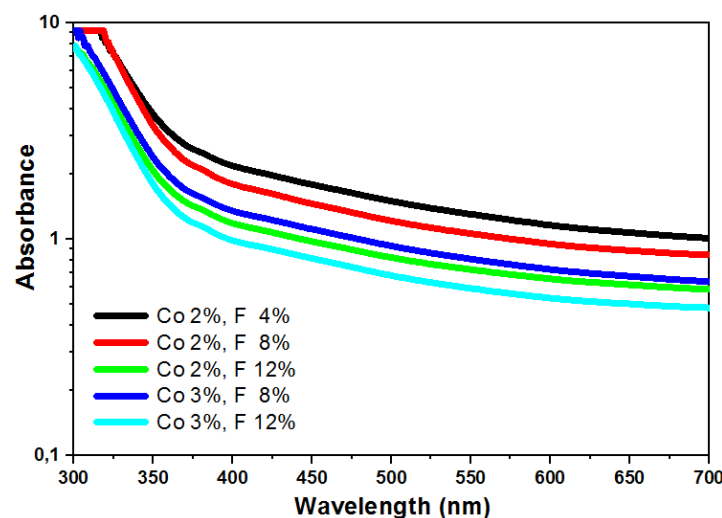


Figure 5. Absorbance spectra of Co and F codoped NiO thin films as a function of Co and F concentrations.

Assuming direct electronic transitions between the valence band and the conduction band, the optical band gap (E_g) of the Co- and F-codoped NiO thin films was determined. The band gap was estimated using Tauc plot method [33], which was constructed from the optical transmittance spectra using the following relations [33,34]:

$$A = \alpha d = -\ln T \quad (4)$$

$$(\alpha h\nu) = B(h\nu - E_g)^n \quad (5)$$

In the above relation, A represents the absorbance, d is the film thickness of prepared thin films; T is the measured transmittance; α denotes the absorption coefficient; B is a constant, $h\nu$ is the photon energy, especially in NiO, $n = 1/2$ for the direct band gap [35] and the band gap energy of Co and F codoped NiO thin films. The optical band gap E was obtained by extrapolating the linear portion of the plot $(A h\nu)^2$ versus $(h\nu)$ to 0 [36], as illustrated in Figure 6(a).

The use of absorbance instead of the absorption coefficient in Equations (3) and (4) is mainly justified by the experimental constraints and the direct proportionality between both quantities for thin films of known thickness. In thin-film optical measurements, the absorption coefficient α is commonly derived from absorbance A using the relation [37]:

$$\alpha = 2.303 \cdot \frac{A}{d} \quad (6)$$

Since the film thickness is known and uniform within experimental uncertainty, absorbance can be directly used as a proportional representation of absorption coefficient without affecting the qualitative interpretation of the optical transitions.

The assumption of allowed direct transitions in Tauc analysis is supported by both previous studies and the experimental results of this work [35]. Literature reports indicate that NiO thin films, whether doped or undoped, often exhibit direct optical transitions in the high-energy absorption region, particularly in nanostructured or thin-film forms. Therefore, the direct transition model is commonly used to estimate the optical band gap of NiO-based materials. In this study, the Tauc plots $(A h\nu)^2$ versus $(h\nu)$ show a clear linear region over a wide photon-energy range, confirming an allowed direct transition. The indirect model does not show comparable linearity, supporting this choice.

The optical transmission data were also employed to evaluate the Urbach energy (E_u) of Co and F codoped NiO thin films using the following relation [37,38]:

$$\alpha = \alpha_0 \exp\left(\frac{h\nu}{E_u}\right) \quad (7)$$

In this expression, α_0 is a constant and E_u represents the Urbach energy. The Urbach energy was determined from the slope of the linear region of the $(\ln A)$ versus photon energy $(h\nu)$ plot [39], as illustrated in Figure 6(b). The logarithm used for Urbach energy determination is the natural logarithm $\ln$ rather than $\log$. This correction may slightly influence the visualization and slope of the linear fitting near the absorption edge, but it does not significantly change the overall trend of the results. The estimated uncertainty in the Urbach energy values is about ± 0.005 eV, which is typical for optical measurements and fitting methods. Therefore, small differences between close values should be interpreted cautiously.

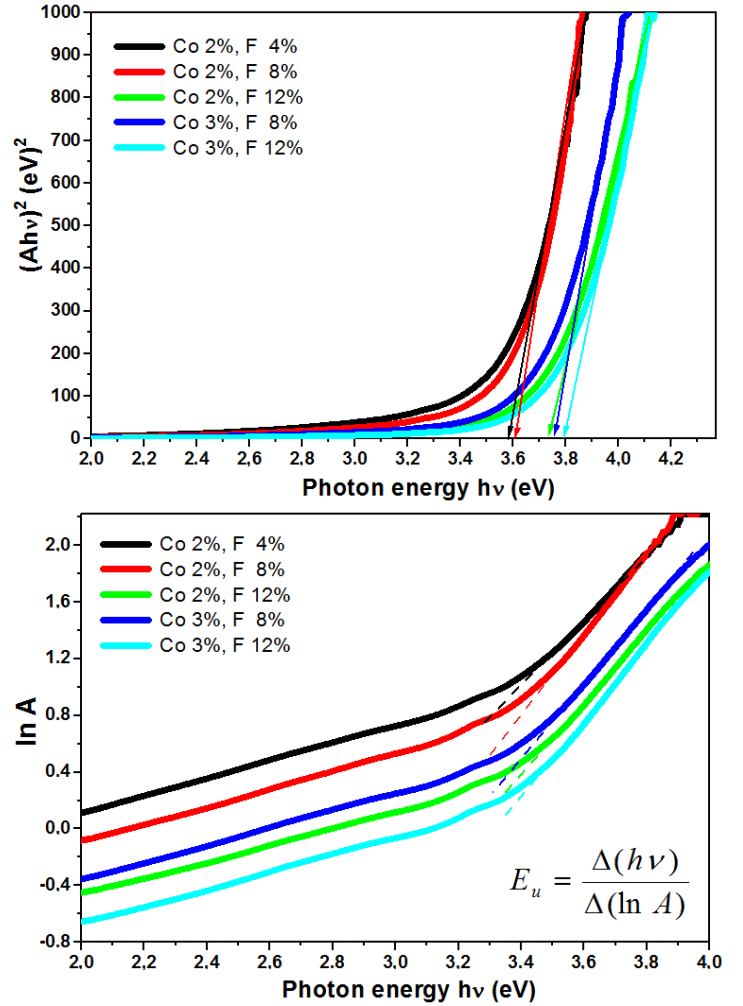


Figure 6. (a): The plot of versus $(h\nu)$ to determinate of optical band gap energy in NiO thin films as a function of Co and F concentrations and (b): The drawn of $(\ln A)$ versus $(h\nu)$ to determinate of Urbach energy in NiO thin films as a function of Co and F concentrations.

Figure 7 presents the variations of the optical band gap (E_g) and Urbach energy (E_u) for Co- and F-codoped NiO thin films at different dopant concentrations. For a constant Co content, the optical band gap increased with increasing F concentration from 4% to 12% and from 8% to 12%. This behavior can be attributed to the substitution of F for oxygen rather than nickel, which minimally perturbs the conduction band compared to metal dopants that replace Ni. Consequently, the many-body effects in the conduction band are reduced, even though the addition of F anions raises the Fermi level by filling previously unoccupied conduction band states in the most heavily codoped samples (2% Co and 12% F or 3% Co and 12% F) [40] (see Table 1). The observed band gap variation is attributed to the combined effect of Co and F codoping, which modifies the electronic structure, carrier concentration, and defect states of the NiO matrix. Dopant incorporation introduces localized energy levels and modifies band tail states, leading to an increase in the optical band gap without forming a new phase, confirming that only the intrinsic NiO transition is observed. The particular behavior observed for the 2%Co-8%F sample is not considered an artifact. It may result from an optimal balance between dopant incorporation,

defect density, crystallinity, and carrier concentration, which can strongly influence the optical transition behavior and absorption edge position.

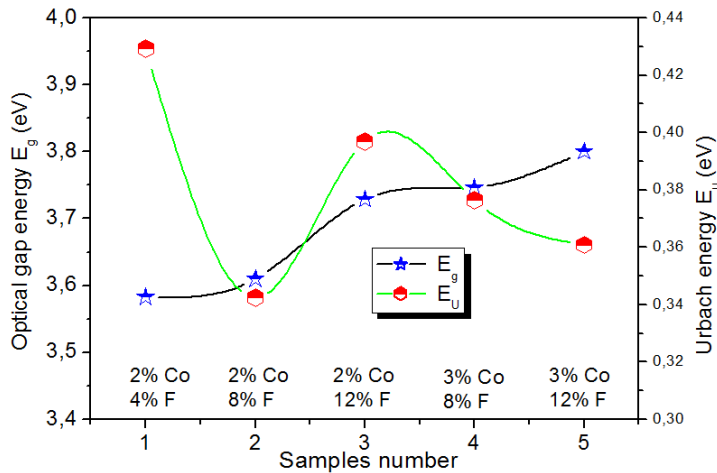


Figure 7. Variation of optical gap energy and Urbach energy of Co and F codoped NiO thin films as a function of Co and F concentrations.

Table 1. Variation of the optical band gap energy E_g and Urbach energy E_u of Co and F codoped NiO thin films.

Co content (%)	F content (%)	E_g (eV) ± 0.005	ΔE_g (eV) ± 0.005	E_u (eV) ± 0.008	ΔE_u (eV) ± 0.008
2	4	3.58	-	0.429	-
2	8	3.61	0.03	0.342	0.087
2	12	3.73	0.12	0.397	0.055
3	8	3.75	0.14	0.376	0.034
3	12	3.80	0.05	0.361	0.015

When the F content is held constant, the band gap also increases with higher Co concentration, e.g., from 2% Co and 8% F to 3% Co and 8% F, or from 2% Co and 12% F to 3% Co and 12% F. This effect is attributed to active electronic transitions involving Co^{2+} 3d levels and the strong sp-d exchange interaction between itinerant sp orbitals of NiO and the localized d orbitals of Co. As a result, the valence band (E_V) narrows downward and the conduction band (E_C) shifts upward, effectively broadening the optical band gap [19].

The minimum Urbach energies of the deposited films were 0.342 eV and 0.361 eV for the 2% Co–8% F and 3% Co–12% F films, respectively. The decrease in Urbach energy with increasing Co and F concentrations is associated with the widening of the optical band gap, which narrows (E_V) and (E_C) while lowering (E_V) and raising (E_C), thereby reducing the density of localized states in the band tails. The variation of the optical band gap is a key property for advanced materials, particularly for applications in visible-light gas sensing based on metal oxide nanostructures. Figure 8 presents the experimental data and linear fit showing the dependence of the optical band gap on Urbach energy. The broadening of the optical band gap in Co- and F-codoped NiO thin films is attributed to the shifting of the conduction band (E_C) upward and the valence band (E_V) downward, which reduces the overlap and effectively increases the energy separation between the bands.

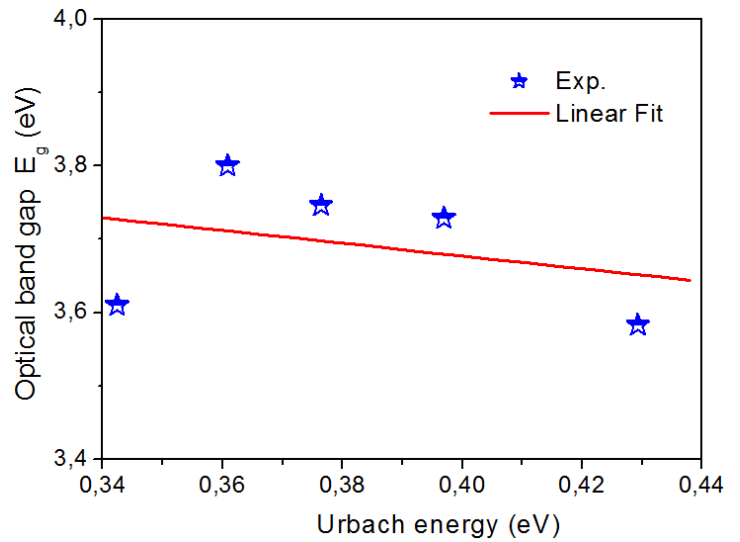


Figure 8. Correlation between optical band gap and Urbach energy of Co and F codoped NiO thin films.

IV. CONCLUSIONS

In this work, Co and F codoped NiO thin films, where $\text{Co/Ni} = 0.02$ and 0.03 , $\text{F/Ni} = 0.04$, 0.08 and 0.12 , were effectively deposited on glass substrates by spray pneumatic approach utilizing nickel chloride hexahydrate, cobalt chloride dihydrate, and ammonium fluoride. The effects of Co and F co-doping on the electrical and optical characteristics of NiO thin films were examined. The electrical properties of Co and F codoped NiO thin films were investigated at different temperatures, which was based on the calculate the voltage and current of the thin films with increase, from 30 to 180 °C and with reduction, from 180 to 30 °C. We have found that the temperature was affected on the electrical properties; the optimum values of voltage were obtained with increase of temperature. The minimum electrical resistivity of the Co and F co-doping NiO films was located at 2%Co and 12%F. The transmission spectra show that the Co and F codoped NiO thin films have the best optical transparent in the visible region. The band gap energy was increased with increasing the Co and F contents in all deposited samples. The minimum Urbach energy was reached at 2%Co and 8%F, it is 0.342 eV.

REFERENCES

- [1] V. Verma and M. Katiyar, *Thin Solid Films* **527**, 369 (2013).
- [2] S. C. Chen, T. Y. Kuo, Y. C. Lin, and H. C. Lin, *Thin Solid Films* **519**, 4944 (2011).
- [3] R. Sharma, A. D. Acharya, S. B. Shrivastava, M. M. Patidar, M. Gangrade, T. Shripathi, and V. Ganesan, *Optik* **127**, 4661 (2016).
- [4] A. Lakel and S. Benramache, *J. Power Technol.* **104**, 201 (2024).
- [5] A. Lakel, S. Lakel, S. Benramache, and O. Belahssen, *J. Chem. Res.* **46**, 17475198211066535 (2022).

- [6] D. Dini, Y. Halpin, J. G. Vos, and E. A. Gibson, *Coord. Chem. Rev.* **304–305**, 179 (2015).
- [7] G. F. Cai, C. D. Gu, J. Zhang, P. C. Liu, X. L. Wang, Y. H. You, and J. P. Tu, *Electrochim. Acta* **87**, 341 (2013).
- [8] A. C. Nwanya, S. U. Offiah, I. C. Amaechi, S. Agbo, S. C. Ezugwu, B. T. Sone, R. U. Osuji, M. Maaza, and F. I. Ezema, *Electrochim. Acta* **171**, 128 (2015).
- [9] R. Romero, F. Martin, J. R. Ramos-Barrado, and D. Leinen, *Thin Solid Films* **518**, 4499 (2010).
- [10] T. Chtouki, L. Soumahoro, B. Kulyk, H. Bougharraf, B. Kabouchi, H. Erguig, and B. Sahraoui, *Optik* **128**, 8 (2017).
- [11] J. Lennox, R. Pepper, W. Martens, V. Gray, J. Alarco, J. MacLeod, and S. Couperthwaite, *Ceram. Int.* **52**, 18024 (2026).
- [12] C. Mrabet, M. Ben Amor, A. Boukhachem, M. Amlouk, and T. Manoubi, *Ceram. Int.* **42**, 5963 (2016).
- [13] R. S. Kate, S. C. Bulakhe, and R. J. Deokate, *Opt. Quantum Electron.* **51**, 319 (2019).
- [14] K. O. Egbo, C. E. Ekuma, C. P. Liu, and K. M. Yu, *Phys. Rev. Mater.* **4**, 104603 (2020).
- [15] W. Yan, W. Weng, G. Zhang, Z. Sun, Q. Liu, Z. Pan, Y. Guo, P. Xu, S. Wei, Y. Zhang, and S. Yan, *Appl. Phys. Lett.* **92**, 052508 (2008).
- [16] X. Chen, L. Zhao, and Q. Niu, *J. Electron. Mater.* **41**, 382 (2012).
- [17] A. Qureshi, A. Mergen, and A. Altindal, *Sens. Actuators B* **135**, 537 (2009).
- [18] Y. Aoun, M. Marrakchi, S. Benramache, B. Benhaoua, S. Lakel, and A. Cheraf, *Mater. Res.* **21**, e20170681 (2018).
- [19] S. Benramache and B. Benhaoua, *Superlatt. Microstruct.* **52**, 807 (2012).
- [20] I. Hotovy, J. Huran, P. Siciliano, S. Capone, L. Spiess, and V. Rehacek, *Sens. Actuators B* **78**, 126 (2001).
- [21] M. Ben Amor, A. Boukhachem, K. Boubaker, and M. Amlouk, *Mater. Sci. Semicond. Process.* **27**, 994 (2014).
- [22] R. Merienne, J. Lynn, E. McSweeney, and S. M. O'Shaughnessy, *Appl. Energy* **237**, 671 (2019).
- [23] M. Ferrara, H. C. Neitzert, M. Sarno, G. Gorrasi, D. Sannino, V. Vittoria, and P. Ciambelli, *Physica E* **37**, 66 (2007).
- [24] M. Mohiuddin and S. V. Hoa, *Compos. Sci. Technol.* **72**, 21 (2011).
- [25] H. L. Chen, Y. M. Lu, and W. S. Hwang, *Surf. Coat. Technol.* **198**, 138 (2005).
- [26] L. Dejam, J. Sabbaghzadeh, A. Ghaderi, et al., *Sci. Rep.* **13**, 6518 (2023).
- [27] M. Obaida, A. M. Fathi, I. Moussa, and H. H. Afify, *J. Mater. Res.* **37**, 2282 (2022).
- [28] I. L. P. Raj, S. Valanarasu, R. S. R. Isaac, M. Ramudu, Y. Bitla, V. Ganesh, and I. S. Yahia, *Optik* **254**, 168634 (2022).
- [29] A. Hakim, J. Hossain, and K. A. Khan, *Renew. Energy* **34**, 2625 (2009).
- [30] S. Moghe, A. D. Acharya, R. Panda, S. B. Shrivastava, M. Gangrade, T. Shripathi, and V. Ganesan, *Renew. Energy* **46**, 43 (2012).
- [31] P. S. Patil and L. D. Kadam, *Appl. Surf. Sci.* **199**, 211 (2002).
- [32] R. Djarallah, B. Benhaoua, and S. Benramache, *Acad. J. Manuf. Eng.* **24**, 170 (2026).
- [33] J. Tauc, R. Grigorovici, and A. Vancu, *Phys. Status Solidi B* **15**, 627 (1966).
- [34] M. Terlemezoglu, O. Surucu, M. Isik, et al., *Appl. Phys. A* **128**, 50 (2022).
- [35] K. Haunsbhavi, D. Alagarasan, N. J. Shivaramu, et al., *J. Electron. Mater.* **51**, 6356 (2022).
- [36] M. Sh. Abdel-wahab, H. K. El Emam, and W. M. A. El Roubay, *J. Mater. Sci.: Mater. Electron.* **34**, 1637 (2023).
- [37] S. Benramache and B. Benhaoua, *Superlatt. Microstruct.* **52**, 1062 (2012).
- [38] R. Sharma, A. D. Acharya, S. B. Shrivastava, T. Shripathi, and V. Ganesan, *Optik* **125**, 6751 (2014).
- [39] K. Sajilal and A. M. E. Raj, *Optik* **127**, 1442 (2016).
- [40] Y. J. Choi, K. M. Kang, and H. H. Park, *Sol. Energy Mater. Sol. Cells* **132**, 403 (2015).

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INFLUENCE OF THE REPULSION OF TWIN IMPACTORS ON GRANULAR CRATERS: PRELIMINARY EXPERIMENTS

INFLUENCIA DE LA REPULSIÓN ENTRE PROYECTILES GEMELOS EN CRÁTERES GRANULARES: EXPERIMENTOS PRELIMINARES

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The formation and morphology of impact craters has been a subject of systematic attention by astronomers and geophysicists for a long time. Impacts may occur in granular terrain, where fluid-like and solid-like phases frequently coexist [1–3]. In fact, *impact cratering* has become a notorious research subject for granular matter scientists over the last couple of decades, especially due to the possibility of studying crater formation and intruder penetration processes by means of relatively inexpensive laboratory experiments [4–9].

Actual craters of geophysical and astronomical interest can be produced by the impact of a single body, but also by multiple impactors in parallel. The so-called “double-craters”, for example, are believed to be caused by the impact of two solid bodies [10]. Those have been reproduced quite convincingly by table-top experiments involving spherical masses impacting a granular bed by Jiménez *et al.*, [11], Kitagawa *et al.* [12] and Yuxuan Luo *et al.* [13] –to the authors’ knowledge. Interestingly, the latter incorporates the fact that two granular intruders interact repulsively with each other as they enter a granular medium [14–17].

The lateral repulsion between intruders can be qualitatively explained by the jamming of grains between intruders [14,18], “re-directing” force chains in such a way that they have a larger lateral component: this situation can be visualized in Fig. 5 of [18].

Here we study the role of repulsive granular interactions in double crater formation from a different angle. We demonstrate experimentally that *repulsion does have a measurable effect in the shape of binary craters* under experimental conditions analogous to those reported in [11,12]. Furthermore, we show that the protocol followed for the preparation of the granular bed plays a crucial role in the output of table-top experiments on doublet craters.

In our experiments, we dropped pairs of 11.0 mm diameter steel beads on the free surface of sand deposited into a cylindrical container (15.5 cm wide and 6.5 cm tall) from a height of 50 cm. The sand was collected at “Santa María” beach

(Havana, Cuba); the grain size was distributed between 0.16 mm and 0.36 mm, peaking at 0.26 mm [19].

Two protocols were followed for the preparation of the sand bed before each dropping experiment. In the first one (POUR-LEVEL) the container was emptied and re-filled by pouring sand from above, slightly surpassing the rim of the container, and then its surface was levelled by horizontally sweeping a plastic ruler. In the second one (POUR-SHAKE) the container was emptied and re-filled by pouring sand from above, and then it was laterally shaken for a few seconds until an even free granular surface was obtained. This implied a more compact granular bed than the one resulting from POUR-LEVEL, but we did not quantify the packing fractions.

Pairs of beads were magnetically released at the same time, side-by-side (i.e. the inter-center distance between the beads was one bead diameter). It is important to note that this minimal initial separation guarantees the immediate emergence of lateral repulsive forces as the impactors touch the granular bed, that would have eventually disappeared if the initial separation was substantially larger [18]. Two bead-pair arrangements were studied: the FREE-TWINS were released without any attachment between the beads (as in [11,12]) while the SIAMESE were glued together by a small lateral area of the spheres. So, while FREE-TWINS could move horizontally relative to each other when touching the granular bed, SIAMESE could not. Ten droppings were performed for each combination of sand filling protocols and bead-pair arrangements, for a total of 40 experiments.

Fig. 1 comprises our basic results. Before discussing it, we should define the aspect ratio of the craters, as:

$$A = \frac{\lambda_{\parallel}}{\lambda_{\perp}} \quad (1)$$

where $\lambda_{\parallel}$ is the edge-to-edge length of the crater along a direction passing by the centers of the two impacting beads,

and $\lambda_{\perp}$ is the edge-to-edge width of the crater perpendicular to the first direction [11]. Both were measured with a 0.05-mm resolution vernier caliper, while shining the craters with an inclined laser sheet in order to facilitate visualization of the craters' edges.

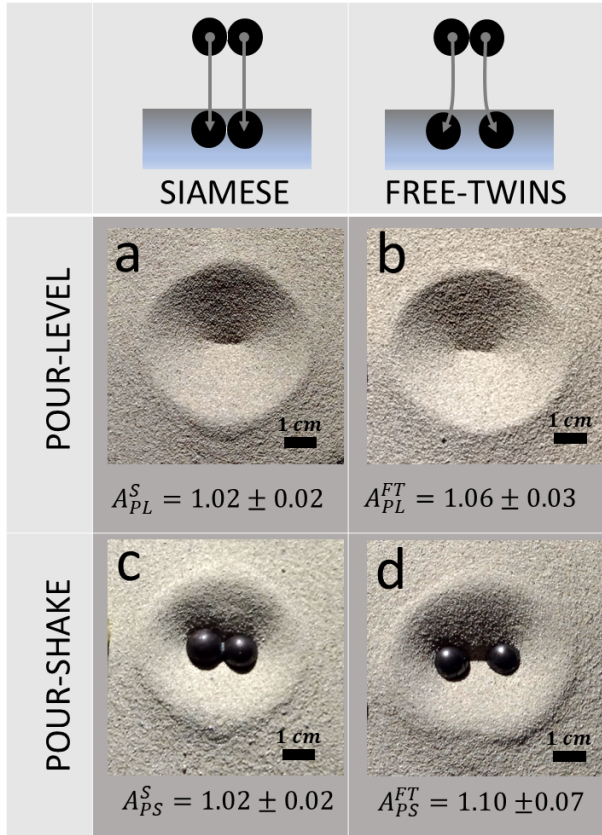


Figure 1. Horizontal repulsion between twin intruders elongates granular craters. (a) Upper panel: image of a crater created by dropping two beads attached to each other from a height of 50 cm on a non-compacted sand bed. Lower panel: Aspect ratio calculated from 10 craters like the one shown in the image (b) Analogous data for craters made by **non-attached** beads on a non-compacted sand bed (c) Analogous data for craters made by attached beads, on a compacted sand bed (d) Analogous data for a craters made by non-attached beds, on compacted sand.

Fig. 1(a) shows the results for the SIAMESE beads dropped on the POUR-LEVEL bed of sand. The upper image shows a picture of a typical crater, taken from top. The image suggests that the crater is quite circular: in fact, the corresponding aspect ratio averaged over 10 repetitions of the experiment gives $A_{PL}^S \sim 1.02$. The situation basically repeats for the case of SIAMESE dropped at a more compacted sand, as illustrated in Fig. 1(c), where $A_{PS}^S \sim 1.02$.

A surprising picture arises when we examine the case of non-attached intruders. Fig. 1(b) reports the results for FREE-TWINS dropped on loose sand resulting from the POUR-LEVEL protocol. The craters are clearly more elongated than for SIAMESE, expressed as $A_{PL}^{FT} \sim 1.06$: as the beads touch the free granular bed, force chains in the region between the intruders are “charged”, in such a way that they push the intruders away from each other [15, 16], resulting in a more elongated crater. The phenomenon is more

clearly revealed for the FREE-TWINS and POUR-SHAKE combination, as illustrated in Fig. 1(d). We hypothesize that here, the more compacted sand bed implies stronger force chains and presumably a larger repulsion force in the horizontal direction, provoking a large gap between the beads (of the order of one bead diameter), which is clearly visible in the snapshot of Fig. 1(d). This results in the largest aspect ratio among the four kinds of experiments: $A_{PS}^{FT} \sim 1.10$. We speculate that this phenomenon has not been reported in previous works because of the use of relatively loose, lower-friction granular packings, where “strong” force chains are less relevant. However, some natural scenarios involve complex, highly compacted granular materials [21].

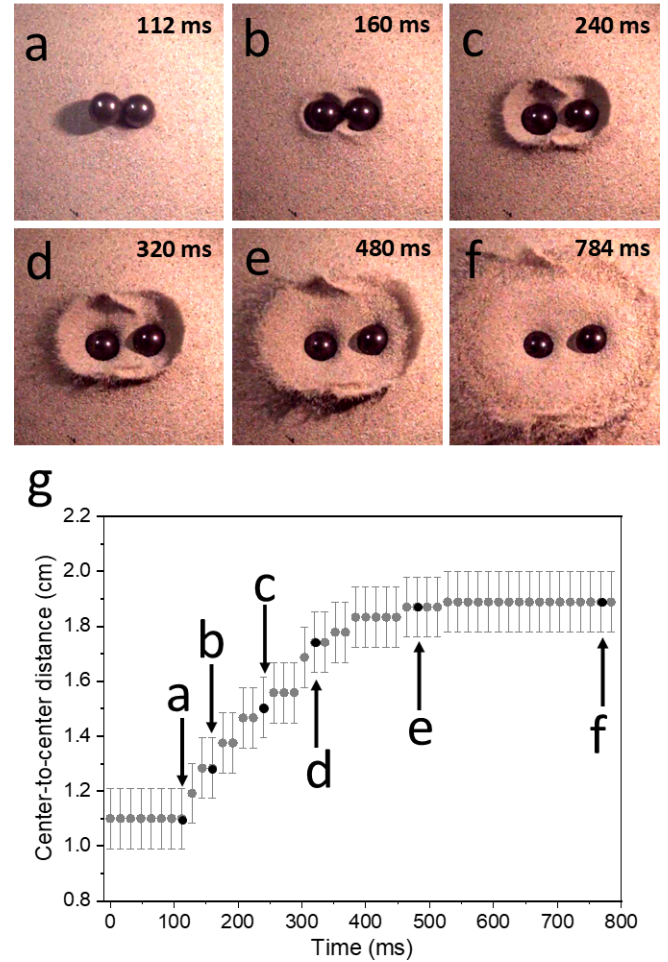


Figure 2. Visualizing twin repulsion during impact cratering. (a)-(f) Snapshots from a video of FREE-TWINS dropped into a sand bed prepared using the POUR-SHAKE protocol. (g) Evolution of the center-to-center bead separation as a function of time based on the same video.

In order to visualize the process of crater formation in the presence of repulsive forces between the intruders, we briefly discuss a video taken at 1000 fps (1920 pixels $\times$ 1080 pixels) of an experiment where FREE-TWINS are dropped on a sand bed prepared by the POUR-SHAKE protocol. The video was taken with a CHRONOS fast camera model CR-21-1.0-32C, using a LAOWA Lens FF 12 mm F2.8 D-Dreamer, at an angle of approximately 30 degrees relative to vertical direction.

Fig. 2 (a) - (f) show snapshots taken from the video and

2 (g) contains a graph displaying the time dependence of the distance between the centers of the beads. In (a), the impactors have not touched the granular surface yet, and the distance between the center of the beads is 11 mm (i.e., one diameter), as shown in (g). In (b), the beads have started to touch the granular surface, and lateral repulsion has already showed up (the inter-center distance is now of the order of 14 mm, as shown in (g)); the outward motion of sand has started. The inter-center distance growth keeps increasing from (c) to (e), until the beads finally remain still and the crater is (almost) completely formed, as illustrated in (f). The maximum inter-center distance between the beads is almost 2 cm, meaning that the gap between the beads approaches one bead diameter.

While Fig. 2 illustrates the role of repulsion for FREE-TWIN impacting POUR-SHAKE, repulsion is also visualized in analogous snapshots taken for FREE-TWIN hitting POUR-LEVEL sand (not shown here).

In conclusion, we have demonstrated that the repulsive horizontal interaction between granular intruders produces a measurable effect in the aspect ratio of the resulting crater, when they are near to each other at the beginning of the impact event. This effect is more notorious when the granular bed is more compact, and is expected to decrease its relevance for looser granular beds, or when the impact energy is very high.

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1. Data availability

The data that support the findings of this study are available from the corresponding author upon reasonable request.

REFERENCES

- [1] H. M. Jaeger, T. Shinbrot, P. B. Umbanhowar, *PNAS* **97**, 12959 (2000).
- [2] E. Martínez, C. Pérez-Penichet, O. Sotolongo-Costa, O. Ramos, K. J. Måløy, S. Douady, E. Altshuler, *Phys. Rev. E* **75**, 031303 (2007).
- [3] A. Baule, F. Morone, H. J. Herrmann, H. A. Makse, *Rev. Mod. Phys.*, **90**, 015006 (2018).
- [4] E. Nelson, H. Katsuragi, P. Mayor, D. J. Durian, *Phys. Rev. Lett.*, **101**(6), 068001 (2008).
- [5] F. Pacheco-Vázquez, J. C. Ruiz-Suárez *Phys. Rev. Lett.* **107**, 218001 (2011).
- [6] H. Torres, A. González, G. Sánchez-Colina, J. C. Drake, E. Altshuler, *Rev. Cubana Fis.* **29**, 1E45 (2012).
- [7] J. C. Ruiz-Suárez, *Rep. Prog. Phys.* **76**, 066601 (2013).
- [8] E. Altshuler, H. Torres, A. González-Pita, G. Sánchez-Colina, C. Pérez-Penichet, S. Waitukaitis, R. Hidalgo, *Geophys. Res. Lett.* **41**, 3032 (2014).
- [9] G. Sánchez-Colina, L. Alonso-Llanes, E. Martínez, A. J. Batista-Leyva, C. Clement, C. Fliedner, R. Toussaint, E. Altshuler, *Rev. Sci. Instrum.* **85**, 126101 (2014).
- [10] K. Miljković, G. S. Collins, S. Mannick, P. A. Bland, *Earth Planet. Sci. Lett.* **363**, 121 (2013).
- [11] M. Jiménez-Valdez, E. Tomay, J. O. Marston, F. Pacheco-Vázquez, *Granular Matter* **24** 115 (2022).
- [12] H. Kitagawa, R. Obara, Yu Masuda, *Phys. Fluids* **37**, 103331 (2025).
- [13] Yuxuan Luo, Xuegang Huang, Chun Yin, Jian Jin, Wenxue Li, Xiao Peng, *Granular Matter* **27**, 80 (2025).
- [14] F. Pacheco-Vázquez, J.C. Ruiz-Suárez, *Nat. Commun.* **1**, 123 (2010).
- [15] V. Diaz-Melián, A. Serrano-Muñoz, M. Espinosa, L. Alonso-Llanes, G. Viera-López, E. Altshuler, *Phys. Rev. Lett.* **125**, 078002 (2020).
- [16] M. Espinosa, V. Diaz-Melián, A. Serrano-Muñoz, E. Altshuler, *Granular Matter* **24**, 2 (2022).
- [17] M. Espinosa, E. Altshuler, *Rev. Cubana Fis.* **39**, 8 (2012).
- [18] J. M. Solano-Altamirano, G. A. Caballero-Robledo, E. Pacheco-Vázquez, V. Kamphorst, J. C. Ruiz-Suárez, *Phys. Rev. E* **88**, 032206 (2013).
- [19] M. Espinosa, L. Martínez-Ortíz, L. Alonso-Llanes, L. A. Rodríguez-de-Torner, O. Chávez-Linares, E. Altshuler, *Sci. Adv.* **9**, eadf6243 (2023).
- [20] F. Pacheco-Vázquez *Phys. Rev. Lett.* **122**, 164501 (2019).
- [21] T. Ishii, A. Kioka, J.-J. S. Huang, T. Tsuji and Y. Yamada, *Phys. Fluids* **37** 023358 (2025).

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A SUPERCONDUCTIVITY BREAKTHROUGH: FEELING THE PRESSURE TO RELEASE THE PRESSURE

UN HITO SUPERCONDUCTOR: SINTIENDO LA PRESIÓN DE RELAJAR LA PRESIÓN

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The discovery of high-temperature superconductivity in cuprates during the late 1980s triggered an intense race to raise the critical temperature (T_c), driven both by scientific pressure and physical pressure applied via diamond anvil cells. While mercury-based cuprates, particularly $\text{HgBa}_2\text{Ca}_2\text{Cu}_3\text{O}_{8+\delta}$ (Hg-1223), held the ambient-pressure record of 134 K for over three decades, achieving higher T_c at ambient conditions remained elusive. This paper reviews the history of pressure-enhanced superconductivity and presents a recent breakthrough: the Pressure-Quench Protocol (PQP). By applying high pressure at room temperature, cooling the sample under pressure, releasing the pressure at cryogenic temperatures (below 20 K), and finally warming to ambient temperature, the high-pressure superconducting phase becomes “kinetically trapped”. This protocol yields an ambient-pressure T_c of approximately 150 K in Hg-1223—the highest ever recorded at ambient pressure. Structural retention is confirmed by synchrotron X-ray diffraction, and the method opens new pathways for discovering and stabilizing high-temperature superconducting phases without requiring continuous external pressure.

El descubrimiento de la superconductividad de alta temperatura en los cupratos durante finales de la década de 1980 desencadenó una carrera intensa por elevar la temperatura crítica (T_c), impulsada tanto por la presión científica como por la presión física aplicada mediante celdas de yunque de diamante. Si bien los cupratos basados en mercurio, en particular el $\text{HgBa}_2\text{Ca}_2\text{Cu}_3\text{O}_{8+\delta}$ (Hg-1223), mantuvieron el récord de 134 K a presión ambiente durante más de tres décadas, lograr T_c 's más altas en condiciones ambientales seguía siendo un desafío. Este artículo revisa la historia de la superconductividad potenciada por presión y presenta un avance reciente: el protocolo de temple por presión (PQP, por sus siglas en inglés). Al aplicar alta presión a temperatura ambiente, enfriar la muestra bajo presión, liberar la presión a temperaturas criogénicas (por debajo de 20 K) y finalmente calentar hasta temperatura ambiente, la fase superconductora de alta presión queda “atrapada cinéticamente”. Este protocolo produce una T_c a presión ambiente de aproximadamente 150 K en Hg-1223—la más alta registrada hasta ahora a presión ambiente. La retención estructural se confirma mediante difracción de rayos X con sincrotrón, y el método abre nuevas vías para descubrir y estabilizar fases superconductoras de alta temperatura sin requerir presión externa continua.

Keywords: Superconductivity, Pressure-Quench Protocol (PQP), Mercury-based cuprates (Hg-1223), Metastable high-pressure phase, Ambient-pressure record critical temperature

The late 1980s and early 1990s were years of extreme pressure for the scientists working in the field of superconductivity.

On the evening of March 18, 1987, during the American Physical Society March Meeting at the Hilton Hotel in New York City, a historic session took place. The discovery of high-temperature superconductivity in the $\text{CuBa}_{0.15}\text{La}_{1.85}\text{O}_4$ “cuprate” in 1986 [1] and in its “cousin” $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ early in 1987 [2] had triggered an unprecedented frenzy. The session room was full of scientists past midnight; researchers slept in the aisles, and others watched on closed-circuit television outside. This event was immediately dubbed the “Woodstock of Physics”—making an analogy with the famous three-day music concert celebrated in 1969.

The community felt the pressure to understand and, above all, to raise the T_c —i.e., the critical temperature above which superconductivity disappears. Bednorz and Müller’s compound $\text{La}_{2-x}\text{Ba}_x\text{CuO}$, $x = 0.15$ had a T_c of 35 K (−238 °C) at ambient pressure, which was rapidly increased while hydrostatic pressure was applied to the material using a diamond anvil [3]. This observation suggested C. W. Chu

and co-workers the creation of the material $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$, that exhibited a critical temperature of 93 K (−180 °C) at ambient pressure. This value of T_c was above liquid nitrogen’s boiling point (77 K), constituting a giant step in terms of “experimental affordability” and potential applications—see Fig. 1.

It can be said that during the late 1980s and early 1990s, the field of superconductivity was driven by pressure: the pressure to find new compounds with higher critical temperatures, and the physical pressure applied by diamond anvil cells. Both served to push higher. *But the holy grail has been always to increase the critical temperature at ambient pressure.* In this article we will present a very recent discovery where a record critical temperature is obtained at ambient pressure. . . by applying hydrostatic pressure!

A SUPERCONDUCTIVITY PRIMER

Superconductivity is a macroscopic quantum state characterized by three fundamental fingerprints. *Zero*

resistance is the most intuitive: below T_c , the DC electrical resistivity drops to practically zero ohms in high-quality samples, limited only by measurement sensitivity. *The Meissner effect* – the *expulsion* of magnetic flux from the interior of a superconducting sample even when the field does not change in time – distinguishes a superconductor from a perfect conductor. *Flux quantization* is perhaps the most direct evidence of macroscopic quantum coherence: in a superconducting ring or a hollow cylinder, the magnetic flux enclosed is quantized in units of $\Phi_0 = h/2e$, where h is Planck's constant, and e is the charge of the electron. This quantization directly reveals that the charge carriers are electron pairs (called Cooper pairs) instead of single electrons, as in common metals [4]. It also demonstrated that superconductivity is a macroscopic quantum state, along with other phenomena, like Josephson tunneling [5].

Cooper pairs are a crucial ingredient of the microscopic theory of conventional superconductivity, known as the Bardeen-Cooper-Schrieffer (BCS) model [6]. Intuitively, BCS works like this: as an electron moves through the lattice of positive ions, it attracts the ions slightly, creating a local positive charge distortion. A second electron is then attracted to this distortion, forming a bound pair – a Cooper pair – even though both electrons are negatively charged and repel each other in the free space. The lattice vibrations (phonons) act as the glue. This pairing is fragile: the pair size (coherence length) can range from a few to hundreds of nanometers, much larger than the interatomic spacing. But once formed, all Cooper pairs condense into the same quantum ground state, allowing them to flow without resistance. However, Cooper pairs can be destroyed in different ways: by increasing temperature, by increasing an applied magnetic field, or by increasing an applied electric current [4].

Copper pairs can be also destroyed by applying mechanical pressure, but sometimes it can make them stronger. An external pressure applied to a superconductor reduces interatomic distances. Within the framework of the BCS mechanism (valid for conventional superconductors), this may strengthen the electron-phonon coupling by increasing the density of states at the Fermi level, thus increasing the critical temperature. For the case of unconventional superconductors like the cuprates –whose precise pairing mechanism is still unknown– pressure may optimize orbital overlap and charge transfer, implying a higher critical temperature [7].

SUPERCONDUCTING MATERIALS: A SAGA OF RECORDS

In 1911, Heike Kamerlingh Onnes accidentally found that mercury became superconducting at 4.2 K [8], for which he received the Nobel prize in Physics in 1913 [9]. For the next seven decades, progress was slow, as seen in Fig. 1. For example, Nb_3Ge reached a record critical temperature of 23 K (approximately six times that of mercury) only in 1973. The so-called “conventional superconductors” (represented with black dots in Fig. 1) are well described by the BCS theory and required liquid helium cooling –a rather expensive

refrigerant, if compared with liquid nitrogen. The landscape changed dramatically in 1986 when Bednorz and Müller discovered superconductivity at 35 K in $\text{CuBa}_{0.15}\text{La}_{1.85}\text{O}_4$, as mentioned above: not only did it establish a record high critical temperature at ambient pressure; it also broke the tradition of metallic or metallic-alloy superconductors. Moreover, C. W. Chu's group increased the critical temperature in the $\text{CuBa}_{0.15}\text{La}_{1.85}\text{O}_4$ system to 40 K by applying pressure: it is believed that this result made him suspect that the perovskite structure with appropriate atomic substitutions had a serious potential for improvement of superconducting properties beyond those of $\text{CuBa}_{0.15}\text{La}_{1.85}\text{O}_4$. He was proved right by the obtainment of the celebrated $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ material, with an absolute record critical temperature of 92 K at ambient pressure, in 1987. Besides being an enormous improvement in the critical temperature, crossing the barrier of 77 K meant that the superconducting state could be attained using the relatively inexpensive liquid nitrogen as refrigerant. These achievements kicked off the frantic race for higher critical temperatures starting in 1987.

Other cuprate superconductors with even higher critical temperatures were soon found: all of them have one structural feature in common: the existence of copper-oxygen layers of atoms, along which superconductivity is strong. Fig. 1 shows the members with higher critical temperature of all the main cuprate families by means of red dots (there also exist non-conventional, non-cuprate superconductors with relatively small critical temperatures that are not included in the graph). Now, we will concentrate on a particular cuprate family: the mercury-based materials.

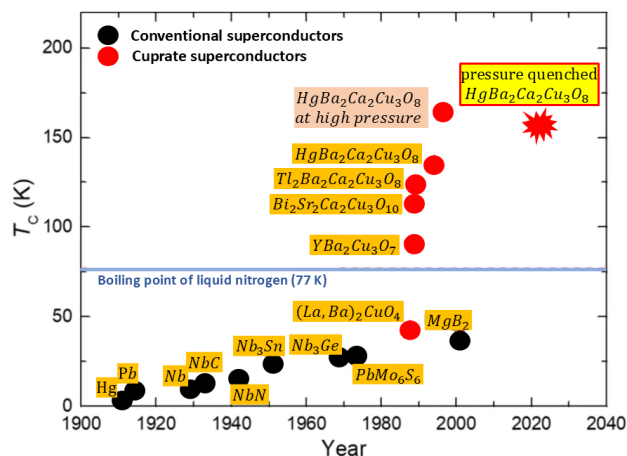


Figure 1. Evolution of the critical temperature in conventional and cuprate superconductors. The chemical formulas shown in the graph for the cuprates are idealized: for example, the actual formula for $\text{HgBa}_2\text{Ca}_2\text{Cu}_3\text{O}_8$ is $\text{HgBa}_2\text{Ca}_2\text{Cu}_3\text{O}_{8+\delta}$, where $\delta < 1$ represents an imperfection in the oxygen stoichiometry, of paramount importance for obtaining superconductivity.

The path to the mercury-based cuprates began in 1993 at two laboratories nearly simultaneously. In Switzerland, a team at the École Polytechnique Fédérale de Lausanne (EPFL) led by S.N. Putilin and E.V. Antipov were exploring the Hg–Ba–Ca–Cu–O system, a hazardous family many avoided due to the toxicity of mercury. Using a high-pressure synthesis

technique to stabilize the structure, they successfully created the first member of a new cuprate family: $\text{HgBa}_2\text{Cu}_3\text{O}_{4+\delta}$. This single-layer compound exhibited a critical temperature of 94 K at normal atmospheric pressure [10]. Almost immediately, a second team led by A. Schilling at ETH Zürich independently confirmed the discovery and reported an even more dramatic result: *a sample of formula $\text{HgBa}_2\text{Cu}_3\text{O}_{4+\delta}$ showed superconductivity approximately at 134 K, an ambient-pressure record that has survived for more than three decades* [11].

Sometime later, the race to unlock that potential was taken up by C.W. Chu's group at the University of Houston. Knowing that pressure was a powerful enhancing tool, from decades of experience, they synthesized the mercury compound $\text{HgBa}_2\text{Ca}_2\text{Cu}_3\text{O}_8$, placed a tiny sample inside a diamond anvil cell and squeezed it to pressures as high as 45 GPa. The effect was remarkable: the atomic layers were forced closer together, optimizing the electronic interactions, and the critical temperature soared to 164 K under pressure, shattering the previous record. This is the highest confirmed critical temperature ever achieved in a cuprate superconductor [12].

The value of the record critical temperature (under pressure) increased in 2015, when the compound H_2S (hydrogen sulfide), under a pressure of 155 GPa, showed a critical temperature of 203 K [13]. This is considered a metallic superconductor, but it is not included in Fig. 1. Finally a compound with a clathrate structure, formed by a network of ten hydrogen atoms with a lanthanum atom at its center (LaH_{10}), subjected to a pressure of 170 GPa, showed superconductivity at temperatures below 250 K (-23°C , almost ambient temperature!) [14].

This search for room-temperature superconducting materials has not been free of controversy. A team led by Ranga Dias at the University of Rochester published an article in 2020 claiming that a carbon-sulfur hydride-based superconductor, when subjected to a pressure of 267 GPa, exhibited superconductivity at 15°C . However, after numerous doubts were raised by several researchers in the field, the article was retracted by *Nature* in 2022, against the authors' wishes, who stood by their claim of having made a valid discovery. In 2023, the same team reported (again to *Nature*) an even more striking result: superconductivity at 21°C and a pressure of 1 GPa in the compound lutetium-nitrogen hydride (N-Lu-H). That same year, the study was retracted by the journal, in an even more concerned turn, as some of the co-authors requested the retraction.

Beyond this case, in 2023 a South Korean team presented online a copper-lead-phosphorus-oxygen alloy (known as LK-99) that was supposedly a superconductor at ambient temperature and pressure, generating excitement and debate on social media. However, the scientific community's failure to replicate the result completely refuted the finding, and it is now known that the anomalies observed in LK-99 were due to the presence of copper sulfide impurities in the sample. We personally owe a lot to the mercury-based cuprates: due to their high critical temperature, our research group was able to experimentally study superconducting phenomena within a relatively wide temperature range, although liquid

nitrogen was the only refrigerant available to us. We were able to systematically measure the hysteresis and relaxation effects typical of ceramic superconductors, demonstrating that polycrystals of nominal composition $\text{HgBa}_2\text{Cu}_3\text{O}_{8+\delta}$ behave as a collection of strongly superconducting grains connected by "weak links" that experience Josephson tunneling [15–18].

QUENCHING THE PRESSURE

While most of the scientists in the superconducting community feel today much less pressure than commonly experienced during the late 1980's and early 1990's, some of the protagonists of that era have kept the feeling alive. That is arguably the case with C. W. Chu.

In a very recent article, his group successfully solved a longstanding problem: how to preserve a high-pressure superconducting phase after the applied pressure is released. They achieved it through a method called Pressure-Quench Protocol (PQP) that was applied to polycrystalline samples of $\text{HgBa}_2\text{Ca}_2\text{Cu}_3\text{O}_{8+\delta}$ (Hg-1223) [19]. It consists of four basic steps, during which the temperature dependence of the sample's resistivity was measured. Here we explain the PQP process:

Step 1 – High-pressure conditioning at room temperature. A Hg-1223 polycrystalline sample is loaded into a diamond anvil chamber with a pressure medium (neon or Daphne oil). The pressure is increased to a value known to optimize the of this cuprate, [12].

Step 2 – Cooling under pressure. While maintaining a high pressure, the anvil chamber is cooled down, and the resistance of the sample is verified in real time using the four-probe method. The black curve in Fig. 2 illustrated the evolution of the resistance for a particular experiment, shown for temperatures above 100 K: a wide transition from the normal state at room temperature (at the right of the curve) to the superconducting state (to the left of the curve) can be seen. The sample was actually taken all the way down to a temperature of 4.2 K, not shown in the graph.

Step 3 – Pressure release at low temperature. This is the critical innovation: instead of releasing pressure at room temperature (which would cause the lattice to relax to the ambient-pressure structure), the anvil chamber is slowly decompressed back to 1 atmosphere while the sample remains below 20 K. This "cold decompression" kinetically "traps" the high-pressure crystal structure because atomic diffusion (the "reordering of atoms") is frozen. For the sample illustrated in Fig. 2, the decompression took place at 4.2 K (not seen in the graph).

Step 4 – Warming to ambient temperature. After full pressure release, the anvil chamber is warmed to 300 K. The retained high-pressure phase remains metastable. The red curve in Fig. 2 shows the superconducting-to-normal transition as temperature was increased after releasing the pressure at 4.2 K. The resulting critical temperature indicated by a vertical arrow in the graph (that should be more properly called onset critical temperature [18]) is approximately 150 K at 1 atm – the

highest ambient pressure ever recorded, breaking the previous record of 134 K [11]. Notice that the figure does not show a superconducting resistivity very near zero ohms, but the data is shown for relatively high temperatures; superconductivity was assessed also using other techniques –especially AC susceptibility.

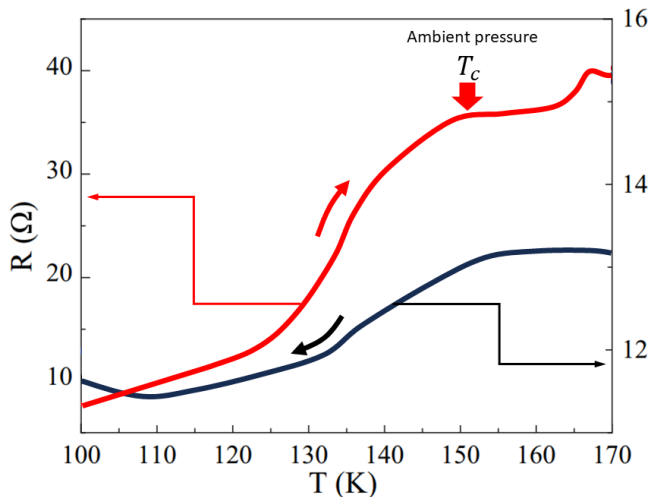


Figure 2. Tracking the sample's resistance during the Pressure-Quench Protocol in real time. The resistivity vs. temperature curves shown correspond to an experiment performed for one $\text{HgBa}_2\text{Ca}_2\text{Cu}_3\text{O}_{8+\delta}$ is $\text{HgBa}_2\text{Ca}_2\text{Cu}_3\text{O}_{8+\delta}$ polycrystalline sample. The horizontal arrows indicate the vertical axis corresponding to each curve (Sketch inspired by Fig.2E of [19]).

Of course, establishing a critical temperature record is a very serious matter, so the authors performed several further studies to crosscheck the results. Structural retention was confirmed by synchrotron X-ray diffraction. Rietveld refinement showed that copper-oxygen bond lengths and apical oxygen positions remain locked in the compressed geometry. Phonon calculations indicated that this geometry increases the electronic density of states at the Fermi level, thereby enhancing the pairing interaction. In addition to these “intrinsic” reasons to explain the improvement in superconducting properties, “extrinsic” factors seem to crucially contribute: the authors speculate that sample imperfections may help “trapping” the strongly superconducting phase after releasing the pressure [19]. The complexity of sample imperfections at many levels and their effects on the superconducting properties have indeed haunted us for decades [15–18], so it is not surprising for us that the precise role of the defects in the process is far from clear in [19]. In any case, the PQP constitutes a breakthrough in the field of superconducting materials.

In an informal encounter with C. W. Chu in 2000, one of us (E.A.) asked him “Professor, where do you think the discovery of room-temperature superconductivity will occur?”. He thought for a couple of seconds, and said “Probably in an unknown, little laboratory somewhere in the world”. After

learning about his own group's Pressure-Quenched Protocol, one may suspect that, after all, Prof. Chu was not exactly right.

REFERENCES

- [1] J. G. Bednorz, K. A. Müller, *Z. Phys. B Condens. Matter* **64**, 189 (1986).
- [2] M. K. Wu, J. R. Ashburn, C. J. Torng, P. H. Hor, R. L. Meng, L. Gao, Z. J. Huang, Y. Q. Wang, C. W. Chu, *Phys. Rev. Lett.* **58**, 908 (1987).
- [3] C. W. Chu, P. H. Hor, R. L. Meng, L. Gao, Z. J. Huang, *Science* **235**(4788), 567–569 (1987).
- [4] M. Tinkham, *Introduction to Superconductivity* (McGraw-Hill, 1975).
- [5] Y. Galperin, *Rev. Cubana Fis.* **42**, 78 (2025).
- [6] J. Bardeen, L. N. Cooper, J. R. Schrieffer, *Phys. Rev.* **108**, 1175 (1957).
- [7] B. Lorenz, C. W. Chu, “High Pressure Effects on Superconductivity” in *Frontiers in Superconducting Materials*, A. V. Narlikar (Ed.), Springer Berlin Heidelberg (2005).
- [8] H. Kamerlingh Onnes, *Comm. Phys. Lab. Univ. Leiden* **122**, 122b (1911).
- [9] H. Kamerlingh Onnes, Nobel Lecture, December 11, 1913 – “Investigations into the properties of substances at low temperatures, which have led, amongst other things, to the preparation of liquid helium”.
- [10] S. N. Putilin, E. V. Antipov, O. Chmaissem, M. Marezio, *Nature* **362**(6417), 226–228 (1993).
- [11] A. Schilling, M. Cantoni, J. D. Guo, H. R. Ott, *Nature* **363**(6424), 56–58 (1993).
- [12] L. Gao, Y. Y. Xue, F. Chen, Q. Xiong, R. L. Meng, D. Ramirez, C. W. Chu, *Phys. Rev. B* **50**, 4260(R) (1994).
- [13] A. P. Drozdov, M. I. Erements, I. A. Troyan, V. Ksenofontov, S. I. Shylin, *Nature* **525**, 73–76 (2015).
- [14] A. P. Drozdov, P. P. Kong, V. S. Minkov, S. P. Besedin, M. A. Kuzovnikov, S. Mozaffari, L. Balicas, F. F. Balakirev, D. E. Graf, V. B. Prakapenka, E. Greenberg, D. A. Knyasev, M. Tkacz, M. I. Erements, *Nature* **569**, 528–531 (2019).
- [15] A. J. Batista-Leyva, R. Cobas, M. T. D. Orlando, C. Noda, E. Altshuler, *Physica C* **314**, 73 (1999).
- [16] E. Altshuler, R. Cobas, A. J. Batista-Leyva, C. Noda, L. E. Flores, C. Martinez, M. T. D. Orlando, *Phys. Rev. B* **60**, 3673 (1999).
- [17] A. J. Batista-Leyva, R. Cobas, E. Estévez-Rams, M. T. D. Orlando, *Physica C* **331**, 57 (2000).
- [18] A. J. Batista-Leyva, M. T. D. Orlando, L. Rivero, R. Cobas, E. Altshuler, *Physica C* **383**, 365 (2003).
- [19] L. Deng, T. Habamahoro, A. Safezoddeh, B. Karki, S. Kazibwe, D. J. Schulze, Z. Wu, M. Julian, R. P. Prasankumar, H. Zhou, J. S. Smith, P. R. Hosur, C. W. Chu, *PNAS* **123**, e2536178123 (2026).

CHARLA DIVULGATIVA DE JOSÉ EDELSTEIN EN LA HABANA: ¿POR QUÉ EL AZAR ES CENTRAL EN LA CUÁNTICA?

“El gran ludópata”, ese fue el título de la charla divulgativa que dio José Edelstein el 9 de enero en la Facultad de Física de la Universidad de La Habana. Primer viernes tras las vacaciones, casi todos los estudiantes habían tenido cuatro largas horas de exámenes finales en la mañana y sin embargo allí estaban en la tarde, llenando por completo el teatro. Y no eran solo estudiantes, en el público había profesores e investigadores de todas las generaciones y campos de la física.

Edelstein es un físico teórico argentino formado en el Instituto Balseiro y doctorado por la Universidad Nacional de La Plata. En la actualidad, es profesor en el Departamento de Física de Partículas de la Universidad de Santiago de Compostela e investigador del Instituto Gallego de Física de Altas Energías (IGFAE), en España. Además de su trabajo en teoría de cuerdas y gravedad cuántica, posee una extensa trayectoria como divulgador. Es autor de libros como “Antimateria, magia y poesía” (2014), “Einstein para perplejos” (2017) y, más recientemente, “Trece maneras de mirar al cielo” y “La tiranía del azar” (ambos de 2025). Para el público más joven, es también una cara familiar en canales de divulgación como Date un Vlog y The Wild Project.

La pregunta que dio título a la charla —¿quién es el gran ludópata?— sirvió de hilo conductor para un viaje por un debate científico histórico: la pugna entre Albert Einstein y Max Born sobre el papel del azar en el universo. Mientras Einstein defendía un cosmos determinista y creía que la mecánica cuántica era una teoría incompleta, con variables ocultas aún desconocidas, Born postulaba que la probabilidad era un elemento fundamental e irreducible de la naturaleza. Edelstein guió a la audiencia a través de este desencuentro, que décadas después se resolvería experimentalmente: los trabajos de Alain Aspect, John Clauser y Anton Zeilinger —galardonados con el Nobel de Física en 2022— confirmaron que la naturaleza viola los límites que implicaría cualquier teoría de variables ocultas locales, dando la razón a la visión probabilística de Born. Hacia el final de la conferencia, Edelstein destacó la lección de fondo: la ciencia avanza mediante la evidencia experimental, no por

autoridad, intuición o elegancia teórica. Einstein, a pesar de sus argumentos poderosos y lógicos, estaba equivocado. Born, con una propuesta que desafiaba el sentido común, tenía razón. Fue el método científico, riguroso y neutral, el que zanjó la disputa.

Para cerrar con un ejemplo fuera de lo común, describió cómo estos mismos principios cuánticos podrían estar operando en el mundo animal: investigaciones recientes sugieren que aves migratorias como el petirrojo utilizan un mecanismo basado en la proteína criptocroma de sus ojos. Al activarse con la luz, esta proteína generara pares de moléculas entrelazadas cuya química sensible al campo magnético terrestre parece actuar como una brújula biológica. Así, el azar cuántico podría estar guiando desde lo invisible el vuelo de un pequeño pájaro.

Al despedirse ante una prolongada ovación, quedó clara la respuesta implícita a la pregunta inicial: el gran ludópata es la propia realidad, que juega con reglas probabilísticas y no deterministas, tal como Born intuyó y los experimentos confirmaron. La charla no solo llenó un teatro, sino que recordó, una vez más, que la mejor divulgación es la que nos enfrenta al asombro de un universo que aún nos depara sorpresas.



El gran Ludópata. José Edelstein (tercero desde la izquierda) junto a estudiantes de pregrado de Física y a la autora (al centro) el día 9 de enero de 2026.

Lic. Cristina Díaz Faloh

Facultad de Física, Universidad de La Habana

CUBA LOGRA TRES MEDALLAS DE BRONCE EN LA OLIMPIADA DE FÍSICA KAIPHO.

La KaIPhO es una olimpiada internacional de Física, organizada por la Universidad de Kazán, ciudad capital de la República de Tartaristán, región semiautónoma de Rusia. La Olimpiada fue convocada a finales de 2025 y celebrada los días 14 y 15 de Mayo de 2026 con formato

presencial y online. A diferencia de otras olimpiadas, la inscripción fue individual. Cuba fue el cuarto país con más participantes registrados, pero solo 26 pudieron concretar su participación online por falta de electricidad o problemas de conectividad. La Olimpiada tuvo como centro de sus temarios

problemas característicos de Física Teórica. Se inscribieron un total de 108 estudiantes de 16 países provenientes de países del continente americano y euroasiático. Los estudiantes cubanos José Ángel Machín Fuentes (oriundo de Santiago de Cuba), así como Sergio Daneel Santiesteban Sarmiento y Mauricio Chinchilla Machado (de La Habana), lograron en tan difícil evento medallas de Bronce. Los dos primeros jóvenes mencionados recién concluyeron el 12mo grado y no matriculan aún la Licenciatura de Física en el Instituto Superior de Ciencias y Tecnologías Nucleares y la Facultad de Física de la Universidad de la Habana respectivamente; Mauricio Chinchilla Machado es estudiante del 11no grado del IPU “Saúl Delgado”. Los tres estudiantes fueron entrenados en la Facultad de Física de la UH.



En plena competencia. Estudiantes cubanos realizando el examen, en modalidad online desde la Facultad de Física de la universidad de La Habana, el 14 de mayo de 2026.

Dr. Saúl Laramendi

Facultad de Física, Universidad de La Habana

ALICE EN EL PAÍS DE LAS MARAVILLAS

Aunque recién hemos conocido sobre esta noticia anunciada en octubre de 2025, no podemos dejar de reportarla. Un grupo de cuatro científicos del Centro de Aplicaciones Tecnológicas y Desarrollo Nuclear (CEADEN) fue galardonado con el prestigioso Premio Breakthrough en Física Fundamental. El premio fue otorgado al proyecto internacional ALICE (A Large Ion Collider Experiment) del CERN, en el que ellos colaboran, y se les reconoció por su labor en la administración del sitio web del proyecto, así como por su participación en

investigaciones relacionadas con colisiones de iones pesados y rayos cósmicos. Los científicos cubanos fueron Ernesto López-Torres, Katherin Shtejer-Díaz, Raúl Arteché-Díaz y Guillermo Mesa-Pérez, como parte de un extenso grupo de investigadores de múltiple países que fueron galardonados, sobre la base de su co-autoría en las publicaciones científicas asociadas a los cuatro experimentos del Gran Colisionador de Hadrones (LHC) del CERN entre 2015 y julio de 2024.

Versión de la noticia aparecida en <https://elbohio revista.com/index.php/2025/10/11/cientificos-cubanos-agradecen-entrega-de-premio-internacional/>

(consultada el 18 de junio de 2026)

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IN MEMORIAM A JUAN GUALBERTO DARIAS GONZÁLEZ

El pasado 8 de marzo de 2026, la comunidad científica cubana perdió a un notable exponente: el Profesor Titular Juan Gualberto Darías González, quien falleció a los 73 años de edad. Graduado de Física en la Universidad de La Habana en 1975, el Prof. Darías dedicó su vida profesional al Centro de Aplicaciones Tecnológicas y Desarrollo Nuclear (CEADEN), institución que dirigió durante cinco años.

Su labor científica, plasmada en publicaciones de alto impacto y patentes, lo consagró como un experimentador excepcional. Su curiosidad intelectual, sin límites, le permitió incursionar con éxito en diversos campos de la física. Realizó contribuciones en la instrumentación óptica, donde diseñó y desarrolló láseres y sensores, y aplicó extensamente la técnica de speckle dinámico al estudio de objetos biológicos para el seguimiento de procesos en microbiología y en tejidos. Los últimos prototipos que ensambló como parte de su trabajo en este tema son todavía utilizados en el Servicio de Cirugía Plástica y Quemados del Hospital Hermanos Ameijeiras. Su pericia también abarcó la espectroscopía de masa MALDI y la creación de servicios especializados de metrología óptica. En la última etapa de su carrera, como miembro del grupo de Nanociencias del CEADEN, el Prof. Darías realizó notables aportes al desarrollo de métodos para la síntesis, purificación, caracterización y aplicación de nanomateriales de carbono.

El impacto de su actividad profesional trasciende sus publicaciones. Fue un formador incansable de nuevas generaciones de científicos, guiando tesis de posgrado e impartiendo cursos de pre y postgrado. Su liderazgo natural lo llevó a integrar y presidir los comités organizadores y científicos de innumerables eventos científicos, entre ellos los congresos de la Sociedad Cubana de Física (de la cual fue Vicepresidente Organizador entre 2011 y 2014), los simposios NURT, TECNOLASER, las Conferencias Internacionales de Aplicaciones de la Óptica y la Fotónica, y los talleres Nanosinergia. Se desempeñó como experto en programas nacionales de investigación, árbitro de revistas científicas, oponente académico en ejercicios de defensa de pregrado y representante de Cuba en el Consejo de la Red Iberoamericana

de Óptica (RIO) y en la Comisión Internacional de Óptica (ICO).



Juan Gualberto Darías González (12 de julio de 1952 – 8 de marzo de 2026)

Su personalidad honesta, integra, bondadosa, modesta y generosa pervivirá en la memoria de todos aquellos que tuvimos la fortuna de compartir su compañía. Al partir deja también una bella familia de hijos y nietos educados e inspirados en su vida ejemplar.

Dr. Luis Felipe Desdín García (CEADEN)

Dra. Ana Ester Cabal Rodríguez (CEADEN)

Dr. Carlos Manuel Cruz Inclán (CEADEN)

Dr. Evelio Ramírez Miquet (Editorial RCF)

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LUIS PÉREZ TAMAYO: UNA VIDA DEDICADA A LA FÍSICA Y SU ENSEÑANZA

Luis Pérez Tamayo nació el 1 de marzo de 1944 en Cacocum, municipio de Holguín de la provincia Oriente, y falleció en la ciudad de Holguín el 15 de abril de 2026, a la edad de 82 años. Se graduó de Ingeniero físico en la Universidad de Oriente en 1971. Obtuvo el grado científico de Doctor en Ciencias Físico-Matemáticas, especialidad de Física Nuclear y Partículas Elementales, en la Universidad Estatal de Leningrado (antigua Unión Soviética), en 1982. Entre 1971 y 1989 desarrolló su trabajo en la Universidad de Oriente, donde fue Jefe del Departamento de Física Nuclear entre 1971 y 1986, y Jefe de Departamento de Investigación y Posgrado en dicha universidad, desde 1987 hasta 1989.

Lideró una investigación en la aplicación de los neutrones a la industria y la minería, en la región de Santiago de Cuba entre 1985 y 1986. Fue jefe del Laboratorio de Vigilancia Radiológica Ambiental de la región oriental de Cuba en la Secretaría Ejecutiva para Asuntos Nucleares (SEAN) de Holguín entre 1989 y 1996. En la SEAN también se desempeñó como Delegado territorial.

En el curso escolar 1996-1997 pasó a la docencia en el Instituto Pedagógico "José de la Luz y Caballero" de Holguín y ocupó la responsabilidad de Jefe del colectivo de Física General, en el Departamento de Física y Electrónica hasta 1998. Al iniciar el curso 1998 se trasladó a la Universidad de Holguín "Oscar Lucero Moya", en el Departamento de Física-Química, donde impartió docencia hasta su jubilación en el 2009, con la categoría de Profesor Auxiliar.

Fue uno de los autores de la investigación del fondo radiológico ambiental cubano, galardonada con el Premio de la Academia de Ciencias de Cuba en 1994.

En el trabajo científico se destacó en la formación de jóvenes, incluidos premios y reconocimientos en foros estudiantiles de ciencia, tecnología y ciencias pedagógicas. Fue tutor de varias tesis de Maestría y de un Doctorado en Ciencias Físicas. Trabajó en cuatro líneas de investigación, y los resultados obtenidos fueron avalados con la publicación de unos 40 artículos científicos en revistas nacionales y extranjeras en temas relacionados con las reacciones nucleares, aplicaciones de los neutrones, radiactividad ambiental, cosmología y enseñanza de la Física. Presentó 35 ponencias en eventos nacionales e internacionales. Escribió textos sobre los Premios Nobel de Física, teoría general de la relatividad y cosmología, la física en el entorno de Félix Varela y cien comentarios actuales sobre ciencia.

Fue miembro fundador del Consejo Asesor Científico Provincial del CITMA en Holguín y miembro del Consejo

Editorial de la revista "Ciencias Holguín". Mantuvo una columna de comentarios científicos en la página web del telediario "Al día" en el canal provincial Tele Cristal. Desde su fundación fue miembro de la Sociedad Cubana de Física.

Desde muy joven se integró a las actividades estudiantiles. Fue fundador de la Asociación de Jóvenes Rebeldes y entre 1960 y 1962 fue presidente de dicha asociación en Holguín. En abril de 1962 participó en el Primer Congreso de la UJC, y entre 1962 y 1964 fue miembro del Buró provincial de dicha organización en Oriente.

En febrero de 2014 se le otorgó, en Holguín, el Premio Provincial de Física "Arnaldo Batista Díaz", por sus aportes significativos en la enseñanza de la Física y a la investigación científica.



Luis Pérez-Tamayo (1 de marzo de 1944-15 de abril de 2026)

Estas notas póstumas pretenden ser portadoras del reconocimiento de la Sociedad Cubana de Física y en especial, del grupo de Holguín a la obra del Doctor Luis Pérez-Tamayo y también de acompañamiento a su familia por la pérdida física de esa prestigiosa personalidad de la física y su enseñanza en Cuba.

Segifredo Luis González-Bello

Departamento de Matemática-Física

Universidad de Ciencias Pedagógicas "Enrique José Varona"

LÁZARO RIGOBERTO BENAVIDES LEONARD (5 DE DICIEMBRE DE 1941-28 DE ABRIL DE 2026)

El ingeniero eléctrico, licenciado en física y Dr. C. Lázaro Benavides comenzó su labor docente como brigadista "Conrado Benítez" en la Campaña de Alfabetización en 1961. Al final la Campaña, matricula en la carrera de Ingeniería Eléctrica de la Universidad de La Habana, de la cual se graduó en 1967. Pero como el mismo confesara en una entrevista, le apasionaba la física, así que se incorporó desde 1962 al movimiento de alumnos ayudantes impartiendo las asignaturas de esa disciplina en carreras de ingeniería. En 1970 cumplió su sueño al graduarse de licenciado en física en la Universidad de La Habana. Esto abrió un camino que siguieron otros profesores, al graduarse de ingenieros.

Al inaugurarse la Cujae, comenzó a impartir clases en ese centro a los estudiantes de nuevo ingreso siendo aún estudiante en la Colina Universitaria hasta que, a finales de 1965, todas las carreras de ingeniería pasaron a la Cujae, integradas junto a Arquitectura en la Facultad de Tecnología. Los departamentos de Física, Matemática, Química e Inglés se habían integrado en la llamada Escuela de Ciencias Básicas, siendo Benavides el jefe del Dpto. de Física durante varios años. Inicialmente el claustro del departamento de Física estaba integrado por estudiantes de ingeniería e ingenieros que se quedaban en este una vez graduados. Gracias a las relaciones establecidas por Benavides se captaron estudiantes de licenciatura en física como alumnos ayudantes que después de graduados se quedaron en el departamento como profesores. Posteriormente, esta misma labor de captación la realizó en el Pedagógico "Enrique José Varona", incorporando doctoras en pedagogía, lo cual resultó en un claustro con una integración de saberes que permitieron perfeccionar el proceso de enseñanza-aprendizaje de la física en las carreras de ingeniería bajo su dirección, siendo esta una época de mucho aprendizaje para todo el claustro. Fue Benavides uno de los autores de libros de textos de Física propios de la CUJAE, que fueron utilizados durante décadas en la formación de ingenieros. Todavía algunos consultamos los libros de Óptica y Física Moderna escritos por Benavides. Fue el primer doctor en ciencias del departamento graduado en la antigua URSS, y abrió las puertas para que otros profesores desarrollaran su trabajo de investigación en Física aplicada en centros de ese país. Se especializó en la enseñanza de la Física en Ingeniería Eléctrica, y se ganó un espacio en el diseño de una nueva asignatura del plan de estudio, Teoría del Campo Electromagnético, de la cual además fue profesor principal y autor del libro de texto que recibió el premio de la crítica científico-técnica de la Academia de Ciencias de Cuba en el año 2015.



Dr. C Lázaro R. Benavides Leonard

En sus últimos años de trabajo dedicó sus horas de investigación a la modelación físico-matemática de procesos vinculado a un proyecto del MINFAR, destacándose por su exigencia y profesionalidad en todas las tareas a él encomendadas.

Integró muy temprano en 1962 las filas de la UJC y más tarde en 1972 las del PCC. En ambas organizaciones ocupó responsabilidades a diferentes niveles. En particular fue secretario general del partido en el núcleo de Ciencias Básicas.

Creó una linda familia con Mirtila, también profesora por muchos años de la Cujae. Su quehacer como docente será siempre recordado por profesores y por los muchos ingenieros que contribuyó a formar.

Gilda M. Vega Cruz

Profesora titular, Honoris Causa

Departamento de Física Universidad Tecnológica de La Habana "José Antonio Echeverría", CUJAE

