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PhD course of National Interest in Technologies for
Fundamental Research in Physics and Astrophysics

Annual report

Name and surname: SAMINA ZUHRA

Cycle and a.a.: Cycle: 40th, 2024/2025

Curriculum: Computing

Supervisors: Prof. Daniele Martello, Prof. Gabriella Cataldi

- **Research activity carried out during the year**

Aim of the Project

The aim of the SABRE-North project is to perform a definitive, model-independent test of the annual modulation signal reported by the DAMA/LIBRA experiment. This goal requires achieving an unprecedentedly low background rate of 0.1 counts per day per kilogram per keV (cpd/kg/keV) in the energy region relevant for dark matter searches. To this end, the project is developing ultra-high purity NaI(Tl) crystals, produced through the zone refining process, in which impurities such as potassium (K) and lead (Pb) are swept toward one end of the ingot for subsequent removal.

Research Activity: Construction of Mathematical Modeling

Our research has focused on developing a mathematical model to predict the distribution of impurities in NaI(Tl) crystals after multiple passes of the zone refining process. The dominant impurities, **K** and **Pb**, accumulate at the *tail end* of the ingot, allowing the purified section to be extracted.

The model incorporates key factors such as:

- Length of the molten zone (W)
- Effective segregation coefficient (k) of impurities
- Initial impurity concentration (C_0)
- Geometry of the ingot (conical + cylindrical shape)
- Number of zone refining passes

The model was designed to track the impurity concentration in the solid phase (C_s) during solidification across different regions of the ingot:

- When the molten zone is at the starting point ($x = 0$) in the conical region,
- As the molten zone progresses step by step along the ingot,
- At the end of the ingot, where normal freezing occurs and solute rejection is maximal,



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iv. After the molten zone exits, leaving the final impurity distribution.

Finding: Using a computational implementation in Mathematica, it is found that after 25 refining passes, the average concentration of potassium impurity in the purified section of the ingot (cut ratio 0.8:0.2, i.e., discarding the last 20% of the ingot) was reduced to ~ 0.096 relative to the initial concentration (normalized to 1).

Challenges Faced

The experimental work in SABRE-North is complex and costly. A major challenge is that the exact segregation coefficients of impurities like potassium and rubidium are hard to determine, and the process is not perfectly uniform across refining passes. To overcome this, we tested our model with different computational tools (Mathematica and Fortran-based computation), and the results matched well, giving us confidence in the approach. In particular, Mathematica proved especially effective for mathematical modeling and graphing, which greatly supported our analysis.

Future Work:

Our next step is to explore the application of machine learning techniques to analyze photomultiplier tube (PMT) waveforms in dark matter experiments.

Modern machine learning methods, such as convolutional neural networks (CNNs), recurrent neural networks (RNNs), and anomaly detection algorithms have shown promising results in improving signal classification, noise reduction, and event reconstruction.

Through this study, I will investigate state-of-the-art machine learning approaches used in PMT waveform analysis that shows their strengths and limitations. The work will involve testing different models on simulated and experimental PMT data to evaluate their performance in identifying rare physics signals.

By comparing traditional pulse-shape analysis with machine learning-based methods, this project aims to contribute to faster and more accurate data processing techniques for detectors.



Explanation:

Zone Refining Process

Zone refining is a purification technique that uses a moving oven to create a molten zone in an impure ingot. Impurities with a segregation coefficient less than 1, like potassium (K), prefer the liquid state and are carried to the terminal end of the ingot. Impurities with a segregation coefficient greater than 1, such as lead (Pb), prefer the solid state and are pushed to the starting end.

$$K_{eff} = \frac{C_s}{C_l}, \quad \begin{cases} K_{eff} < 1 \text{ (for K impurities)} \\ K_{eff} > 1 \text{ (for Pb impurities)} \end{cases}$$

By repeating this process, impurities are concentrated at either end of the ingot, allowing for the isolation of a highly pure central section.

Mathematical Modeling of Zone refining:

To construct the numerical model of Zone refining process, non-dimensional parameters are adopted for the ingot. $L=1$, $W/L < 1$, $X = x/L \leq 1$, $M=W/dx$

Where L: Total length of ingot, W: Width of molten zone (0.1), M: Element (Partition) of the molten zone such that $Mdx=W$, X: Normalize distance from the starting of the ingot, A: Cross-section area with $1/20L$ width of Ingot, and C_0 : The uniform initial concentration in the ingot. The effective redistribution coefficient for the impurity segregation is define as,

$$K_{eff} = \frac{k}{(1-k)e^{-v\delta/D} + k},$$

v : moving rate of oven, δ : diffusion boundary thickness,

D : impurity diffusion coefficient

(1)

After n-Passes through Zone Refining

Mathematical model is distributed according to different regions of the crystal,

Region 1:

At $x = 0$,

$$C_s^n(0) = \frac{Kdx}{V(x)} \left(\sum_{i=1}^{L_c} C_s^{n-1}(x) \cdot A(x) + \sum_{i=L_c+dx}^W C_s^{n-1}(x) \cdot A \right)$$

(2)

Region 2:



$$At \quad 0 < x < L_c < L - W,$$

$$C_s^n(x) = C_s^n(x - dx) + \frac{Kdx}{V(x)} \left(C_s^{n-1}(x + W - dx) \cdot A - C_s^n(x - dx) \cdot A(x) \right) \quad (3)$$

Region 3:

$$At \quad L_c < x < L - W,$$

$$C_s^n(x) = C_s^n(x - dx) + \frac{Kdx}{W} \left(C_s^{n-1}(x + W - dx) \cdot A - C_s^n(x - dx) \cdot A \right) \quad (4)$$

Region 4:

$$At \quad L - W < x < L$$

$$C_s^n(x) = 1 + A \cdot dx \left(\frac{1 - K_{eff}}{1 - x} \right) C_s^n(x - dx) \quad (5)$$

Region 5:

$$x = 1$$

$$C_s^n(x) = C_0 / A \cdot dx - \sum_{x=0}^{L-dx} C_s^n(x) \quad (6)$$

Where,

$$A(x) = \frac{x^2}{Lc^2}, \quad V(x) = W - \frac{2}{3} L_c + (1 - A(x) / 3) x$$

Results and Discussion

Fig 1 shows fractional position runs from the head to the tail. For $k = 0.5$ (potassium), the impurity is rejected by the solid and moves with the melt, so the bulk of the ingot is cleaner and a strong spike appears at the tail. For $k = 1.1$ (Pb), the impurity prefers the solid; the profile stays near the initial level through most of the ingot and then **drops** near the tail, showing depletion there.

Fig 2 displays, with more passes ($1 \rightarrow 20$), impurity levels decrease across most of the ingot, while the tail spike becomes sharper and moves closer to the very end. The “**with tip**” (conical end) curves sit slightly below the “**without tip**” curves through most of the length, indicating a small but consistent gain in purification of the useful bulk. The benefit is most visible at low to moderate pass counts and is negligible near the tail, where material is cut away.

In Fig 3: Average impurity falls rapidly in the first few passes and then shows diminishing returns beyond ~ 10 – 15 passes. The “with tip” series is lower than “without tip” at the same pass number, showing a modest advantage for including a conical tip. Additional passes



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beyond the knee of the curve give only marginal improvement, so the optimal strategy is to choose a pass count in this knee region and remove a fixed tail fraction (e.g., 10–20%) where the spike resides.

Practical implications.

- For impurities with $k < 1$, zone refining efficiently moves them to the tail for removal.
- Most of the gain is achieved in the early passes; plan cut lengths and pass counts accordingly.
- A conical tip is a low-cost design choice that slightly improves the purity of the retained bulk.

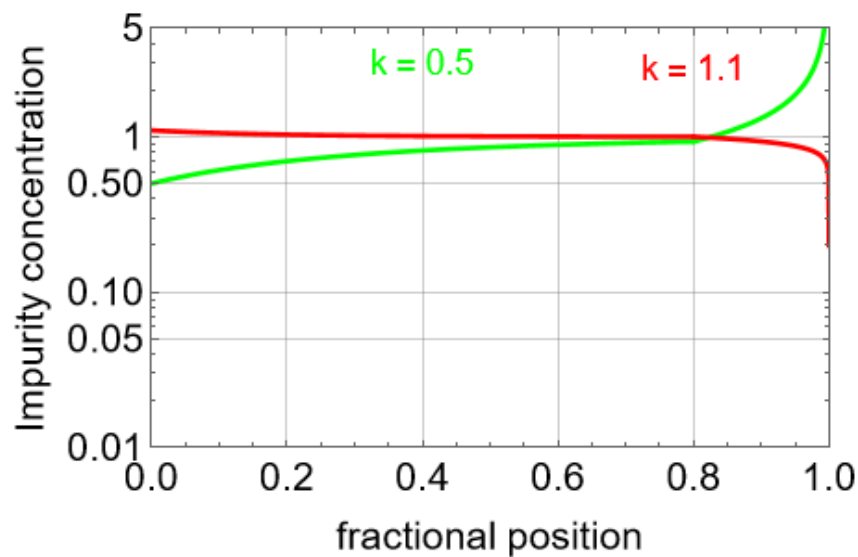
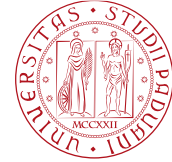


Fig 1: For $K=0.5$, and $K=1.1$ in 1st Pass



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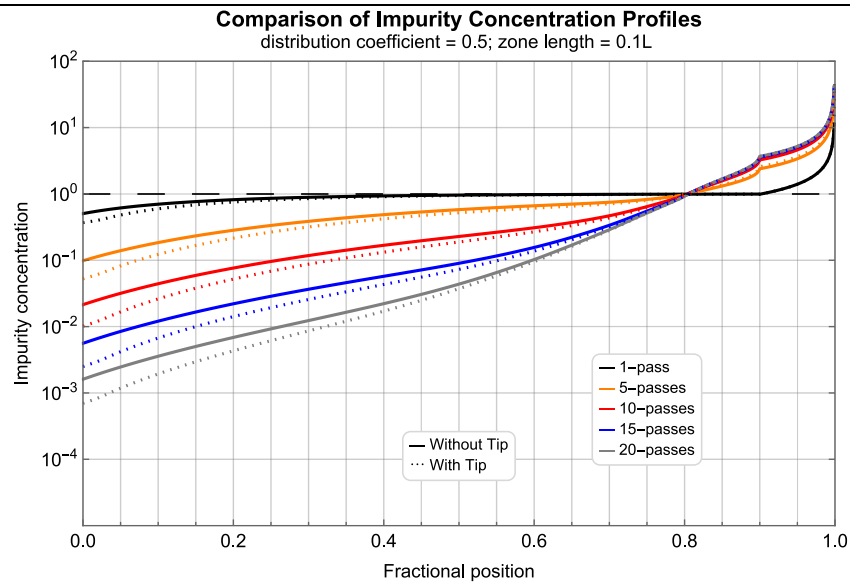


Fig 2: Impurity concentrations in different passes.

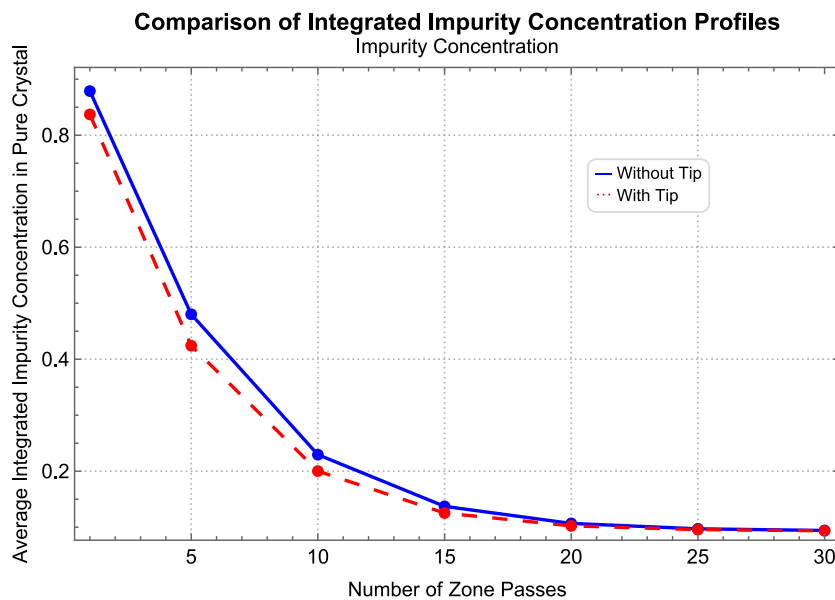


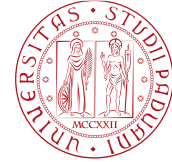
Fig 3: Average concentration at different passes.

Conclusion

Our results demonstrate that zone refining is highly effective for removing impurities from NaI crystals when the segregation coefficient $k < 1$ or $K > 1$. The impurity is efficiently



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driven toward the tail, which can then be removed. Most of the purification occurs within the first 10–15 passes, but by 25 passes the average impurity level in the usable section of the ingot reaches a very low fraction of the starting concentration. In practice, cutting off the final 20% of the crystal, where impurities accumulate, ensures that the remaining 80% achieves the required high purity. The addition of a conical tip provides a modest improvement, but the dominant gains come from repeated passes and tail removal. Overall, 25 passes combined with a 20% tail cut are sufficient to produce ultra-high purity NaI(Tl) crystals for low-background applications.

- **List of attended courses and passed exams**

1. **Cloud Computing and Big Data**

Period: Nov 25th-Jan 23rd, 2025

Duration: 30 hours of lessons (3 CFU)

Instructor: Prof. Tommaso Cucinotta

Category: **Passed**

2. **Neural Networks and Deep Learning: Deep Network**

Period: 4 -26 Feb, 2025

Duration: 20 hours of lessons

Instructor: Prof. Giorgio Buttazzo

Category: **Passed**

3. **Neural Networks and Deep Learning: Advance Topics**

Period: 4th March-02 April, 2025

Duration: 20 hours of lessons

Instructor: Prof. Giorgio Buttazzo

Category: **Passed**

4. **Neural Networks and Deep Learning: Implementation Issues**

Period: 8th April-22nd May, 2025

Duration: 30 hours of lessons

Instructor: Prof. Giorgio Buttazzo



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Category: **Passed**

5. Machine Learning for Physics

Period: 7th March-6 Jun 2025

Duration: 30 hours of lessons

Instructor: Prof. Pierluigi BORTIGNON

Category: **Passed**

6. Quantum AI

Period: 7th April-9th April, 2025

Duration: 10 hours of lessons

Instructor: Prof. Filippo Caruso

Category: **Passed**

7. Big Data Modeling

Period: 8th July-22nd July 2025

Duration: 10 hours of front lessons

Instructor: Prof. Ester Pantaleo

Category: **Exam left**

8. Academic English course

Period: 18 March-8th May, 2025

Duration: 30 hours of front lessons

Instructor: Prof. Angelica Leone

Category: **Passed**

9. CORSO COMUNICATIVO A1 (Italain Course-A1 level)

Period: 8 sep- 19 sep 2025

Duration: 30 hours of front lessons

Instructor: Prof. Cristina Capuzzo

Category: **Passed**



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10. Sicurezza informatica – BASE

Date: 10 March

Category: **Passed**

- **List of attended conferences, workshops and schools, with mention of the talks presented**

1. **2-Weeks School: ISAPP 2025 Lecce:**

Period: 9-20 Jun, 2025

Agenda: "High-energy cosmic rays as messengers: from space to the ground"

Presentation: Flash introduction

Presentation: **Poster** (SABRE-North Experiment for Dark Matter detection)

2. **Five-day School: Gran Sasso National Laboratory (LNGS) (TECH-FPA PhD Retreat 2025)**

Period: 17 - 21 Feb, 2025

- **List of published papers/proceedings**

NIL

- **Thesis title (even temporary)**

*"Applications of Machine Learning in the Analysis of Photo-Multiplier
Waveforms"*

Date: 9/26/2025

Signature...

Seen, the supervisor