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APPLICATIONS OF X-RAY DIFFRACTION (XRD) ANALYSIS IN FORENSIC EXAMINATION

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Abstract
This article analyzes the potential applications of X-ray diffraction (XRD) methods in forensic examination. XRD stands out for its high accuracy, non-destructive analysis, and reproducibility in determining the phase composition of crystalline substances. The study demonstrates the effectiveness of XRD in identifying and comparing forensic materials such as explosives, soil, paints, and pharmaceutical products. Based on international experience and practices in Uzbekistan, the article highlights the reliable use of this method as evidence in judicial and investigative processes. The results confirm the significant scientific and practical value of XRD technology in forensic expertise.

Keywords: X-ray diffraction, phase composition, identifying and comparing forensic materials, fire-technical expertise, short-circuits, crystal lattices.

1. Introduction

Precision, reliability, and scientific validity are of paramount importance in forensic examination [1-8]. Particularly, there is a high demand for methods that provide accurate results in the phase analysis of complex or unknown substances [1,2]. XRD is widely used in forensic laboratories such as the FBI (USA), BKA (Germany), and NFI (Netherlands). In Uzbekistan, research and forensic examinations using XRD are conducted at the Republic Forensic Examination Center named after X. Sulaymonova.

From this perspective, X-ray diffraction (XRD) occupies a special place as a modern analytical method. It allows for non-destructive analysis of the composition of crystalline materials, separation of mixtures, and presentation of results based on international standards.

Paint, soil, dust, and pigment residues found at crime scenes help establish a link between the scene and suspects [3]. Analysis of crystalline oxides and salts in residues from explosion sites enables identification of explosive materials (e.g., ammonium nitrate, barium nitrate) [4]. The crystalline phase and quantitative composition of pharmaceutical products can be determined by XRD, distinguishing genuine products from counterfeits.

This article reviews the directions of XRD application in forensic examination, its advantages, and practical experiences.

2.Research Methodology

XRD is a method used to study the internal structure of crystalline materials. The research process involves the following stages:

Sample Preparation: For analysis, a sample of approximately 10 to 50 mg in the form of crystals or powder is sufficient.

Diffraction Analysis: The samples are analyzed using a modern diffractometer (Malvern Panalytical Empyrean 3).

Data Analysis: The obtained diffraction reflections are compared with international databases (PDF, ICDD) to identify the constituent phases.

Interpretation of Results: Phases, their quantitative ratios, crystal size, deformations, and mixtures are determined.

This methodology is carried out in accordance with forensic examination requirements and based on international standards such as ASTM E3294-22.

3. Results and Discussions

According to the research findings, the XRD method demonstrated high efficiency in forensic examination in the following cases:

3.1 Identification of Unknown Substances

The phase composition of crystalline materials was determined, for example, quartz, calcite, hematite, corundum, and others. This allows conclusions to be drawn about the origin of the substance.

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Below is the diffractogram of a sample submitted to the Fire-Technical Expertise Laboratory of the Republican Center for Forensic Examination named after Kh.Sulaymanova (Fig.1.). The sample was a transparent stone with a light pinkish color and some gray areas. According to the analysis results, it was found to consist of compounds such as SiO_2, Si, Fe_2O_3, and TiO_2 (Tab.1.), confirming that the stone is quartz. The rutile (TiO_2) needles formed as an independent phase within the quartz, imparting golden, reddish, or gray hues depending on their quantity. Fe_2O_3 gives red, reddish-brown, or pink coloration. Based on these observations, it can be concluded that the research was conducted correctly.

3.2 Short Circuits in Electrical Wires

In fire-technical expertise, it is determined whether short circuits in electrical wires occurred before the fire or during the fire [9].

It is well known that the transmission and distribution of electrical energy to buildings, structures, residential houses, transport systems, installations, and similar objects are carried out through conductors. The normal operation of these conductors largely depends on their quality and proper maintenance. If either of these conditions is not met, it may lead to emergency situations in the electrical network, including incidents such as fires and other failures.

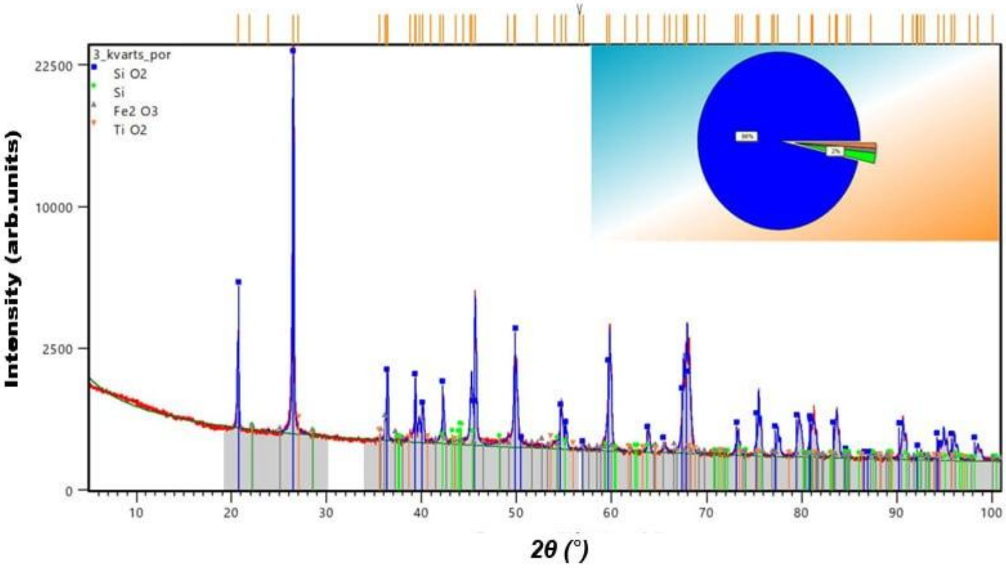

Figure 1. XRD pattern of the sample presumed to be quartz.

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Table 1. Pattern list of the sample

Card Number	Compound Name	Chemical Formula	Mass Fraction, %
01-089-8937	Silicon Oxide	SiO_2	96.0
01-089-9055	Silicon	Si	2.0
01-085-3771	Iron Oxide	Fe_2O_3	1.0
01-080-2545	Titanium Oxide	TiO_2	1.0

In most cases, emergency situations in electrical networks are associated with short-circuit events. While XRD analysis is commonly used in forensic examinations, it can also be effectively applied in the investigation of fire-related incidents and electrotechnical objects.

The use of the XRD method enables the detection of signs of short circuits on electrical conductors recovered from fire scenes and allows for the determination of whether these faults occurred before or during the fire. This method provides high-precision and rapid results, demonstrating its effectiveness in such investigations. Consequently, it becomes possible to determine whether the cause of the fire was related to a short circuit in the electrical wiring or not.

The differences between undamaged sections of aluminum and copper wires and those that have been exposed to high temperatures, subjected to short circuits prior to a fire, or experienced short circuits during a fire are studied by comparing their diffraction patterns [10].

Using XRD patterns, the structural changes in copper (Fig.2.) and aluminum electrical wires caused by varying levels of oxygen exposure, high temperatures, and the effects of short circuits are studied, including the deformation of their crystal lattices (Tab.2.). This approach makes it possible to investigate and differentiate the timing of short circuit occurrences in electrical conductors.

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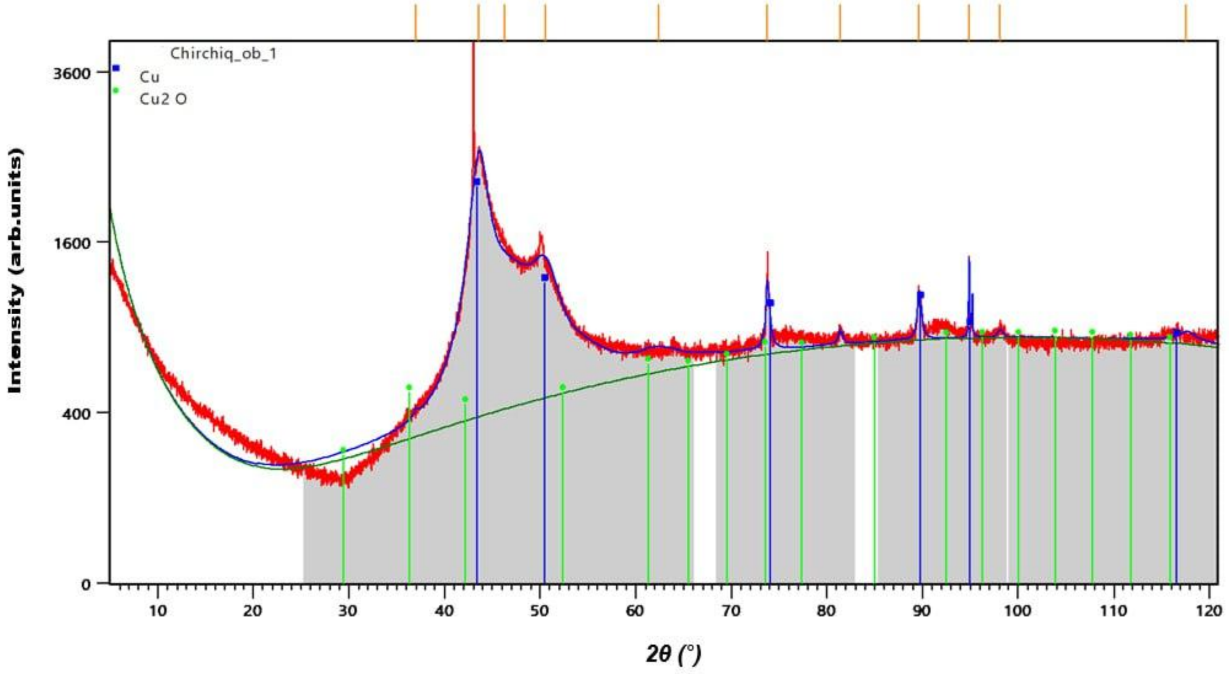

Figure 2. XRD pattern of a copper wire sample subjected to thermal effects caused by a short circuit.

Table 2. Peak list of copper wire sample diffractogram

2θ (°)	Intensity	FWHM [°2θ]	Interplanar spacing [Å]
36.9696	23.83	0.3852	2.42956
43.5556	1058.94	2.3215	2.07623
46.2460	423.35	8.1115	1.96151
50.5754	428.54	4.6970	1.80329
62.3202	71.47	7.2020	1.48870
73.7541	421.70	0.3301	1.28362
81.3405	89.11	0.2637	1.18198
89.5899	310.99	0.3103	1.09329
94.8958	615.52	0.0951	1.04566
98.0615	37.48	0.6415	1.02018
117.5970	60.27	2.4405	0.90057

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Table 3. Pattern list copper wire sample diffractogram

Card Number	Compound Name	Chemical Formula
01-070-3038	Copper	Cu
01-077-0199	Copper Oxide	Cu_2O

4. Conclusion

The study demonstrated the following advantages of XRD technology for forensic examination:

- The sample is preserved and can be reused for other analyses;
- A sample size of up to 10 mg is sufficient for analysis;
- Stable and reproducible results are obtained in each analysis;
- The quantity and type of each crystalline phase in mixtures can be determined;
- The methodology complies with international standards (e.g., ASTM).

Thus, the XRD method in forensic examination allows for:

- Objective and scientifically grounded conclusions;
- Use as reliable evidence in judicial and investigative proceedings;
- High accuracy (up to 0.0001) in the identification and comparison of crime-related materials.

The ongoing development and application of this method in Uzbekistan's forensic practice signify a successful integration of scientific approaches and international experience in the field.

Acknowledgements

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