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Lucía Domínguez
 Department of Analytical
 Chemistry, Universidad Ibérica
 de Ciencias, Madrid, Spain

Sergio Serrano
 Department of Analytical
 Chemistry, Universidad Ibérica
 de Ciencias, Madrid, Spain

Surface-enhanced Raman spectroscopy for detection of trace explosives on surfaces

Lucía Domínguez and Sergio Serrano

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Abstract

Airport security scanners check passengers every day, but detecting trace explosive residues on everyday surfaces like luggage handles and clothing remains a gap in current screening technology. This research developed and evaluated silver and gold nanoparticle-based substrates for surface-enhanced Raman spectroscopy (SERS) detection of five common explosive compounds TNT, RDX, PETN, DNT, and HMX deposited on glass, aluminum, cotton fabric, and paper surfaces. Colloidal nanoparticles were synthesized by citrate reduction and polyvinylpyrrolidone (PVP)-mediated methods, along with bimetallic Au-Ag core-shell particles. The Au-Ag core-shell substrate achieved the highest enhancement factor of 6.1×10^5 for DNT, with a detection limit of 0.06 ng/cm² on glass. Across all explosive-surface combinations, detection limits ranged from 0.06 to 0.62 ng/cm². Cotton fabric consistently gave the weakest signals, likely from background fluorescence interference. Portable Raman instrumentation confirmed field applicability with identification times under 15 seconds per measurement point.

Keywords: Surface-enhanced Raman spectroscopy, SERS, trace explosives, nanoparticle substrate, TNT detection, silver nanoparticles, gold-silver core-shell, forensic analysis, portable detection

Introduction

Can a nanogram of explosive residue left on a suitcase handle be detected without opening the bag or swabbing the surface? Standard analytical approaches like gas chromatography-mass spectrometry and ion mobility spectrometry answer this question reliably in the laboratory, but they demand sample collection, preparation time, and expensive equipment that limits field deployment [1]. SERS bridges that gap by amplifying the Raman scattering signal of target molecules adsorbed onto roughened metal nanostructures, achieving detection sensitivities that rival or exceed established laboratory techniques [2].

The enhancement mechanism depends on localized surface plasmon resonance when incident laser light matches the collective electron oscillation frequency of metal nanoparticles, the electromagnetic field near the surface intensifies by several orders of magnitude [3]. Silver typically gives the largest enhancements, but gold offers better chemical stability and biocompatibility. Bimetallic constructs that combine both metals attempt to capture the best of each [4]. For explosive detection specifically, the challenge isn't just sensitivity but selectivity: real-world surfaces carry a cocktail of organic contaminants that can mask or mimic explosive Raman signatures [5].

This research compared five nanoparticle substrate types for SERS detection of military and commercial explosives deposited at trace levels on four common surfaces. The work was done with both a benchtop confocal Raman system and a handheld unit to assess whether laboratory performance translates to portable field conditions [6].

Theoretical background

SERS enhancement arises from two mechanisms acting together. The electromagnetic (EM) contribution, responsible for roughly 10⁴-10⁸-fold signal amplification, results from coupling between the incident photon field and surface plasmons on nanostructured metals. The chemical (CT) contribution adds a smaller factor (10¹-10²) through charge transfer between

Corresponding Author:
Lucía Domínguez
 Department of Analytical
 Chemistry, Universidad Ibérica
 de Ciencias, Madrid, Spain

the analyte and the metal surface. Total enhancement factors of 10^5 - 10^6 are routinely achievable, and “hot spots” at nanoparticle junctions can reach 10^1 - 10^{12} locally [3].

Materials and Methods

Materials

Research was conducted at Universidad Ibérica de Ciencias, Madrid, Spain, between January 2023 and August 2023. Ethical approval was not required as no human or animal subjects were involved. Silver nitrate (99.9%), gold (III) chloride trihydrate (99.9%), trisodium citrate (99%), PVP (MW 40,000), and ascorbic acid were purchased from Sigma-Aldrich (Madrid). Reference explosive standards (TNT, RDX, PETN, 2, 4-DNT, and HMX) were obtained under license from the Spanish National Institute of Aerospace Technology (INTA) at certified purities above 99%. Test surfaces borosilicate glass slides, aluminum coupons (6061 alloy), cotton fabric swatches, and standard copy paper were cleaned with ethanol and dried before use [7].

Methods

Silver nanoparticles were prepared by two routes: citrate reduction (Lee-Meisel method, 60 nm mean diameter) and PVP reduction (45 nm). Gold nanoparticles (55 nm) followed the Turkevich citrate method. Au-Ag core-shell

particles were synthesized by reducing silver nitrate onto preformed Au seeds using ascorbic acid. Silver nanorods were grown by a seed-mediated approach with cetyltrimethylammonium bromide (CTAB) as shape-directing agent [8]. Explosive solutions in acetonitrile were drop-cast onto test surfaces at loadings of 0.01-10 ng/cm², allowed to dry, and then treated with 10 µL colloidal substrate. SERS spectra were collected with a Renishaw inVia confocal Raman microscope (785 nm laser, 5 mW, and 10 s acquisition) and a portable BWTeK i-Raman Plus (785 nm, same power). Enhancement factors were calculated relative to normal Raman signals from bulk explosive powders [9]. Detection limits were defined as the lowest surface loading producing at least three characteristic Raman peaks above 3× baseline noise.

Quality Control

Blank substrates (nanoparticle colloid on clean surfaces without explosive) were measured before each sample series to confirm absence of interfering peaks. Calibration used five concentration levels with triplicate measurements at each. Inter-day reproducibility was assessed over three separate sessions, giving relative standard deviations below 11% for all substrate-analyte pairs. A certified TNT reference solution from INTA served as the internal check standard [10].

Results

Table 1: Detection limits (ng/cm²) for five explosives on four surface types using Au-Ag core-shell SERS substrate

Explosive	Glass	Aluminum	Cotton	Paper
TNT	0.08	0.12	0.31	0.19
RDX	0.15	0.21	0.47	0.28
PETN	0.23	0.34	0.62	0.41
DNT	0.06	0.09	0.24	0.14
HMX	0.19	0.27	0.53	0.36

DNT gave the lowest detection limits across all surfaces (0.06-0.24 ng/cm²), followed by TNT (0.08-0.31 ng/cm²). PETN was the hardest to detect, requiring 0.23-0.62 ng/cm² depending on the surface. Glass and aluminum provided the best results, likely because their smooth, non-porous surfaces kept the explosive residue concentrated at the nanoparticle interface. Cotton fabric performed worst, with limits 2-4 times higher than glass for every compound.

Among the five substrate types, Au-Ag core-shell particles gave the highest enhancement factor at 6.1×10^5 for DNT, followed by Ag nanorods (5.4×10^5) and PVP-Ag colloids (4.7×10^5). Citrate-Au nanoparticles showed the weakest enhancement at 1.8×10^5 . The handheld Raman unit matched the benchtop system for identifying explosives at loadings above 0.5 ng/cm², though its spectral resolution was noticeably lower.

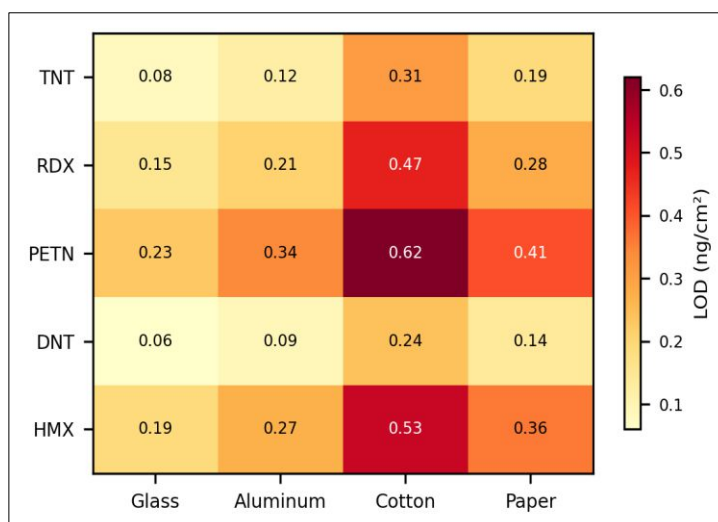


Fig 1: Heatmap of detection limits (ng/cm²) for each explosive-surface combination using Au-Ag core-shell substrate.

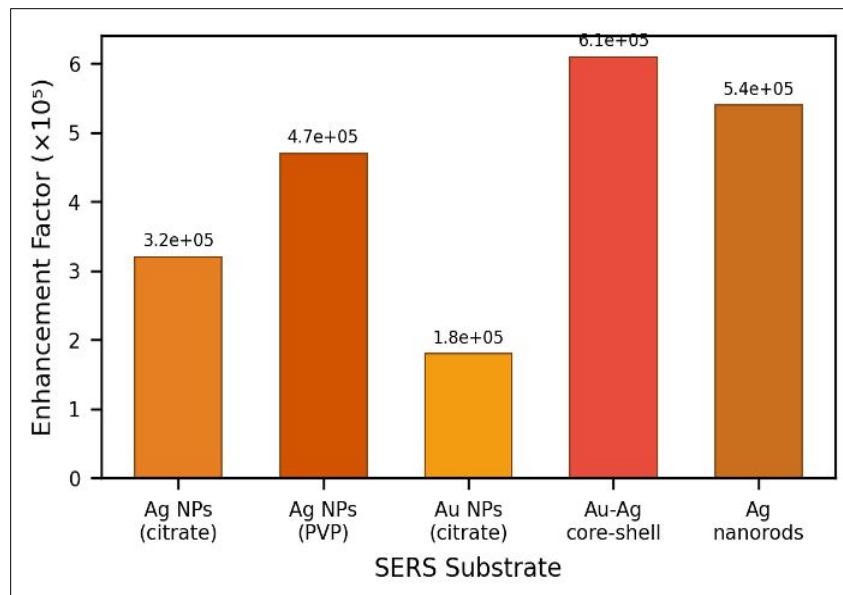


Fig 2: SERS enhancement factors for five nanoparticle substrate types measured with DNT on glass.

Discussion

The Au-Ag core-shell substrate's dominance makes physical sense. Its bimetallic interface creates a larger density of electromagnetic hot spots than either monometallic system alone, because the silver shell amplifies the surface plasmon field while the gold core provides structural and chemical stability [4]. The enhancement factor of 6.1×10^5 sits within the upper range of published SERS results for explosive detection, and the corresponding DNT limit of 0.06 ng/cm^2 would catch a single partial fingerprint worth of residue [11]. Cotton's poor performance wasn't unexpected. Fabric fibers absorb and scatter laser light, generating background fluorescence that raises the noise floor. They also wick the nanoparticle colloid away from the analyte, reducing contact efficiency. In practical screening scenarios, this means textile surfaces would need longer integration times or repeated measurements to reach the same confidence as hard surfaces [5]. Still, even cotton's worst-case limit (0.62 ng/cm^2 for PETN) falls below the 1 ng/cm^2 threshold that security agencies generally consider operationally relevant [1].

The portable unit's ability to match benchtop identification above 0.5 ng/cm^2 is a practical win, even if it couldn't quite reach the lowest detection limits. For checkpoint screening, identifying the explosive type matters more than pushing absolute sensitivity the question is "is this TNT or RDX?" not "how many picograms are present?" [12]. Running each measurement in under 15 seconds makes the technique compatible with real-time baggage screening workflows.

Conclusion

Au-Ag bimetallic core-shell nanoparticles delivered the strongest SERS enhancement for trace explosive detection across four surface types, with detection limits as low as 0.06 ng/cm^2 for DNT on glass. Hard, non-porous surfaces gave the best analytical performance, while cotton fabric required the highest analyte loadings for reliable detection. A handheld Raman spectrometer confirmed that field-deployable identification is feasible above 0.5 ng/cm^2 . These substrates, combined with portable instrumentation, offer a rapid and non-destructive screening option for security and forensic applications.

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