Data Article

Dataset of the synthesis parameters to deposit YSZ on stainless steel AISI 316L by sputtering technique

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ABSTRACT

The data presented in this article are related to the research previously published “improvement of adhesion and barrier properties of biomedical stainless steel by deposition of YSZ coatings using RF magnetron sputtering”. It contains the structural, morphological, compositional and electrochemical characterization of bare AISI 316L substrate which was used as a substrate to coat with yttria-stabilized zirconia (YSZ). The chemical composition and topography analyses from X-ray photoelectron spectroscopy (XPS), Auger electron spectroscopy (AES) and micrographs from atomic force microscopy (AFM) as well as the roughness value of the YSZ-sputtered coating on AISI 316L substrates are presented as complementary data of the article.

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Specifications Table

| Subject area         | Material sciences |
|----------------------|-------------------|
| More specific subject area | Coatings for biomaterials |
| Type of data         | Figures and Micrographs |
| How data was acquired | X-Ray diffraction (Phillips X’Pert diffractometer), scanning electron microscopy (SEM) (JEOL JSM 5300), Electrochemical analysis (GAMRY (600 series) potentiostat/ galvanostat), Atomic force microscopy (AFM), High resolution scanning electron microscopy (HRSEM) (JEOL-6701F), X-ray photoelectron and Auger electron spectroscopies (AES-XPS PHI-548 spectrometer). |
| Data format          | Raw and analyzed |
| Experimental factors | Before the data acquisition from XRD, SEM/EDS and electrochemical, 316L stainless steel substrate was ground up to 1500 grid SiC paper, polished, cleaned with water, ethanol in an ultrasonic bath. YSZ ceramic coatings were deposited on in a Tourus Kurt Lesker Coating System (1 × 10−6 Pa) with argon chamber (20 sccm) at 50 mm (substrate-target distance) from 50 to 250 W and 30 to 120 min [1]. |
| Experimental features | Bare AISI 316 stainless steel substrate and YSZ sputtered on AISI 316L substrate were analyzed. |
| Data source location | CICATA IPN Unidad Altamira, Tamaulipas, Mexico. |
| Data accessibility   | Mendeley Data https://doi.org/10.17632/k2njhtt479.3 |
| Related research article | Z.E. Sánchez-Hernández, M.A. Domínguez-Crespo, A.M. Torres-Huerta, E. Onofre-Bustamante, J. Andraca Adame, H. Dorantes-Rosales, Improvement of adhesion and barrier properties of biomedical stainless steel by deposition of YSZ coatings using RF magnetron sputtering, Materials Characterization 91 (2014) 50-57. |

Value of the Data

- This data can be valuable for comparing the deposit based on YSZ on similar systems to stainless steel.
- The data show the structural, morphological and electrochemical characterization as well as the elemental analysis on the basis of understanding the features of AISI 316L substrate before being sputtered with YSZ.
- It is useful to understand how the topography and morphology of the YSZ deposited on AISI 316L can change as the power is modified from 100 W to 250 W.
- The data can be highlighted with the elemental composition investigations of other type of synthesis.

![Fig. 1. XRD patterns of AISI 316L substrate.](image-url)
1. Data

In this work, a dataset related to the study reported in Ref. [1] to deposit YSZ and delay the corrosion of bare AISI 316L substrate is presented [2–4]. The Fig. 1 corresponds to the diffraction peaks and their intensities data in $2\theta$ angles and counts (a diffractogram) recorded from the sanded and polished

![Fig. 2. SEM micrographs of AISI 316 substrate.](image)

![Fig. 3. EDS of AISI 316 substrate.](image)

| Table 1: Comparison between the nominal and the typical composition of AISI 316 substrate. |
|----------------------------------|----------------------------------|
| Element | AISI 316 Wt. % | Nominal Wt. % |
| Fe      | 69.41          | 66–68          |
| Cr      | 15.58          | 16–18          |
| Ni      | 11.7           | 10–14          |
| Mo      | 1.66           | 2–3            |
| Mn      | 1.6            | 0–2            |
| Si      | 0.66           | 0–1            |
surface of AISI 316 L. These experimental data, acquired as described in the next section, showed the specific crystallographic planes. The data information acquired, detected and processed from secondary electrons by atoms from the AISI 316L surface and excited by the electron beam are shown in the SEM micrographs of Fig. 2. Analyzed area in SEM, seen in Fig. 3, was used for registering the acquisition lines. They were proportional to the elemental composition of the same substrate; their composition of specifically the analyzed area (in wt.%) can be observed and compared to the typical composition in Table 1.

Fig. 4a corresponds to the processed thermodynamic data from cathodic current vs electrode potential \( E_{\text{CCE}} \) over the time in NaCl and PBS. Also, it can be observed the Nyquist plots of the impedance data in NaCl and PBS (Fig. 4b), Bode and phase angle plots for the AISI 316L substrate immersed in 3 wt.% NaCl (Fig. 4c) and PBS (Fig. 4d) and their fittings of these the experimental data.

The morphologies from the processed secondary electrons data in SEM images of sputtered YSZ coatings on AISI 316 L substrate at 100 W, 150 W and 250 W after 120 min of deposition are observed in Fig. 5. Similarly, the morphologies from SEM that were obtained for the substrate coated at 200 W with 100× to 10000× objectives are shown in Fig. 6.

The topography resulting from the surface evaluated from sputtered YSZ coatings on AISI 316 L via AFM analysis at different deposition time (30, 60, 90 and 120 min) and power (200 W and 250 W) are shown in AFM images of Fig. 7 and Fig. 8. From those topographic micrographs, the average surface roughness (Ra) and root mean square average (Rq) data were processed and registered in Table 2.

Auger and low resolution XPS spectrum are shown in Fig. 9a and Fig. 9b, respectively. The peak fitting from XPS corresponding to the oxygen, yttrium and zirconium into YSZ are presented in Fig. 10a–c.

![Fig. 4](image-url)  
Fig. 4. (a) Open circuit potential \( E_{\text{CCE}} \) evolution, (b) Nyquist and (c,d) Bode diagrams of the substrate before coated with YSZ. The measurements were evaluated in a 3 wt. % of NaCl and PBS solutions.
Fig. 5. SEM micrographs from sputtered YSZ coating on AISI 316L substrate synthesized at a) 100 W, b) 150 W, c) 200 W, d) 250 W after 120 min of deposition time.

Fig. 6. SEM micrographs acquired for the coating of YSZ (200 W and 120 min) on stainless steel AISI 316L substrate.
Fig. 7. AFM images of YSZ coatings on AISI 316L at 100 and 150 W.
Fig. 8. AFM images of YSZ coatings on AISI 316L at 200 and 250 W. For comparison, it is also shown the roughness of metallic substrate.
2. Experimental design, materials, and methods

2.1. Data acquisition of AISI 316L substrate

AISI 316L substrate in disk shape of 2.54 cm and 0.4 cm in diameter and thickness, respectively, was characterized to get the structural data by X-Ray diffraction in a Phillips X’Pert diffractometer using monochromatic Cu Kα radiation (\(\lambda = 1.5405 \text{ Å}\)) at 45 kV and 40 mA, step size of 0.02°, step time of 0.5 s. Data were collected at room temperature in the 2θ range of 20°–80° using gracing incidence configuration (θ = 1.1°).

The morphological data to process micrographs of AISI 316L substrate were acquired by scanning electron microscopy (SEM) using secondary electrons in a JEOL JSM 5300 equipment with a Tungsten (W) cathode at a scale of 1 μm and 1 μm. The area inspected from SEM was selected to acquire the data and construct an energy-dispersive X-ray spectrum of its surface; the microscope was equipped with a NORAN Model 5300 EDS analyzer to evaluate the elemental composition (wt.%).

| Sample            | Ra (nm)    | Rq (nm)  |
|-------------------|------------|----------|
| AISI 316 L        | 9 ± 2      | 19 ± 2   |
| 50 w–30 min       | 14 ± 2     | 19 ± 3   |
| 100 w–30 min      | 27 ± 3     | 33 ± 4   |
| 150 w–30 min      | 40 ± 2     | 54 ± 3   |
| 200 w–30 min      | 34 ± 2     | 45 ± 3   |
| 250 w–30 min      | 26 ± 2     | 34 ± 3   |
| 100 w–60 min      | 49 ± 0.7   | 7 ± 1    |
| 150 w–60 min      | 20 ± 2     | 25 ± 3   |
| 200 w–60 min      | 19 ± 3     | 25 ± 5   |
| 100 w–90 min      | 26 ± 3     | 34 ± 5   |
| 150 w–90 min      | 21 ± 3     | 26 ± 3   |
| 200 w–90 min      | 24 ± 6     | 30 ± 5   |
| 100 w–120 min     | 19 ± 2     | 24 ± 1   |
| 150 w–120 min     | 17 ± 2     | 22 ± 3   |
| 200 w–120 min     | 19 ± 2     | 24 ± 2   |
| 250 w–120 min     | 24 ± 6     | 30 ± 5   |

Table 2: Data of average surface roughness (Ra) and the root mean square average of the Z ordinates (Rq).

Fig. 9. (a) Auger spectrum and (b) Low resolution XPS spectrum of YSZ coatings on silicon substrate.
The electrochemical data of bare 316L steel substrate were obtained by open circuit potential (EOCP) and electrochemical impedance spectroscopy (EIS) in a GAMRY (600 series) potentiostat/galvanostat. Analysis was carried out in an electrochemical cell consisting of three electrodes: a graphite bar as counter electrode, saturated calomel electrode SCE (0.2415 V vs SHE) as a reference electrode and the sample as work electrode, (exposed area of the sample was 1.32 cm²). The test was performed under immersion into two mediums: sodium chloride (NaCl) solution and a physiological solution (PBS, 8.0 g L⁻¹ NaCl, 0.2 g L⁻¹ KCl, 0.2 g L⁻¹ KH₂PO₄, 1.15 g L⁻¹ Na₂HPO₄, pH 7.4) during 900 s.

2.2. YSZ coatings on AISI 316L substrate

The morphology data to confirm the nucleation and growing process of YSZ on AISI 316L substrate was processed by SEM using a HRSEM JEOL-6701F. SEM was also used to confirm that the cracking did not extend to the surface of the substrate, different samples were prepared to obtain the data at different magnifications from 100× to 20000×. Topographical features and roughness data of different regions of samples (YSZ coatings on AISI 316L) were acquired by atomic force microscopy (AFM) in a Nanoscope III equipment using an area of 25 mm² and silicon cantilevers under the tapping mode. The data obtained for average surface roughness (Ra) and the root mean square average of the Z ordinates (Rq) were processed with the WSxM 5.0 Develop 2.0 software (Nanotec, Inc.) to acquire the value.

Data from the chemical compositions of the coating, the YSZ on AISI 316L, was obtained from Auger X-Ray spectroscopy in-situ in a AES-XPS spectrometer PHI-548 [5].

Also, data corresponding to the chemical composition of the YSZ coating was obtained by X-ray photoelectron spectroscopy (XPS) using a step energy of 100 eV (low resolution) and 50 eV (high resolution). Samples were coated after exciting the samples by an monochromatized Al Kα line at 1486.6 eV. The working pressure was of 1.9 × 10⁻¹⁰ Pa. The energy scale was calibrated using thick films.
of copper with line at 932.67 eV for Cu 2p\(^{3/2}\). Survey scans were obtained in the 1205-(–10) eV energy interval at 1.0 eV per step, pass energy of 100 eV. Additionally, the high-resolution XPS scans were completed at 0.2 eV energy steps and pass energy of 50 eV (constant pass energy mode). The measured full-width half-maximum (FWHM) for the Cu 2p\(^{3/2}\) line in metallic state with these settings was 1.6 eV. These detailed scans were recorded for the Y3d, Zr 3d, C 1s and O 1s for the coated samples. The analyzed area of the XPS measurements was 800 \(\mu^2\).

From high resolution spectrum corresponding to the YSZ coatings on silicon substrate, the atomic concentration was calculated by using the area under the curve for each transition of Zr, Y and O, and the effective sections of photoionization. Equation (1) was used:

\[
X\% = \frac{\sum_{i=1}^{N} A_X}{\sum_{i=1}^{N} S_X}
\]

where \(X\) is the relative atomic concentration of the element, \(A_X\) is the area under curve of each element \(S_X\) is the sensibility factor.

After calculation, spectra are adjusted by Least Squares method and using Gaussian function.

Deconvolution of spectrum was carried out using the spectral data processor (SDP) software v4.1. The O1s level was deconvoluted into two main peaks at 532.942 eV and 533.323 eV (Fig. 10a). Yttrium deconvolution from spectrum shows the 3d\(^{5/2}\) (159.805) and 3d\(^{3/2}\) (161.885), as doublet.

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Conflict of interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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