Early stages of corrosion of stainless steel 309 S in geological brines studied by sychrotron radiation photoelectron spectroscopy

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ARTICLE INFO

Keywords:
Synchrotron radiation photoelectron spectroscopy
Austenitic steel 309 S
Corrosion mechanism
Radioactive waste disposal
Native oxide
Geological brines

ABSTRACT

The chemical transformations of the native oxide on stainless steel 309 S prior to pitting in anoxic near saturated geological Q3-brine were investigated by synchrotron radiation photoelectron spectroscopy (SRPES). A Cr-rich hydrated mixed iron-chromium-oxide exhibiting n-type semiconducting behavior is formed after wet polishing. Surface accumulation of holes in the metastable pitting potential region induces the hydroxylation of oxide bonds and a subsequent selective dissolution of iron. The open structure of the remaining surface chromium hydroxide facilitates the inward access of chloride and water. The inhibiting effect of sulfate is ascribed to the formation of stabilizing O-S-O bridges blocking chloride access.

1. Introduction

The corrosion of stainless steel in hot anoxic saturated geological brines has deserved a large interest in the repository research, since salt domes are being considered as a possible host for high-level radioactive waste [1,2]. Stainless-steel 309 S is used for the manufacturing of inner vessels in several container designs [3] because of the keeping of its mechanical strength at the high temperatures generated by irradiation after sealing of the repository. Upon an eventual intrusion of groundwater, the development of an anoxic and wet environment with a high salinity at temperatures near the condensation point is expected. The oxygen trapped in the repository is consumed by reaction with surrounding minerals, by microbial activity [4] or during corrosion of the outer carbon steel vessel.

The corrosion resistance of austenitic stainless steels upon immersion in aqueous solutions is ascribed to the formation of a chromium-rich oxide film [5,6]. Hydroxides and bound water predominate at the outermost part of the passive layer whereas oxides are rather formed at the film-substrate interface [5,7]. The higher concentration of Cr^{III} in the passive film was attributed to the higher dissolution of Fe^{III} in the aqueous phase [8,9]. This hypothesis was demonstrated by angle resolved XPS and ToF-SIMS studies reported by Tardio et al. [10]. They indicate that when 316 L stainless steel is cleaned by ion bombardment before to be exposed to the air, a mixed oxide is formed with amounts of Fe^{III} and Cr^{III} proportional to their concentration in the alloy. The Cr^{III} enrichment occurs only after immersion in water with a simultaneous increase of hydration water and hydroxide at the outermost part of the oxide. ToF-SIMS studies of passivation in sulfuric acid solutions reported by Wang et al. [11], on the other hand, revealed the formation of a mixed Cr^{III}-Fe^{III} hydroxylated oxide with a bi-layered structure: a highly enriched chromium oxide in the inner layer and a predominant iron hydroxide in the outer layer.

The surface chemistry of the native oxide and its transformation upon exposition to chloride containing solutions play an essential role in the nucleation and growth of pits. Albeit the role of Cl^- in the nucleation of pits is matter for discussion [12,13], it is generally accepted that the arrival of chloride at the bare metal surface is a *sine qua non* requisite for the stabilization of an already nucleated pit in stainless steel [14]. This implies an adsorption of Cl^- as a triggering first step for the pitting nucleation [15–18] which can be counteracted by oxyanions such as SO_4^{2-}, NO_3^- and ClO_4^- [19].

In this paper, a model experiment consisting in the polarization of a steel sample in a saturated geological brine using an in-system electrochemical cell attached to a synchrotron radiation photoelectron spectroscopy (SR-PES) facility is presented. This new approach attempts to elucidate the surface chemical changes which induce the pitting of stainless steel in this specific environment.

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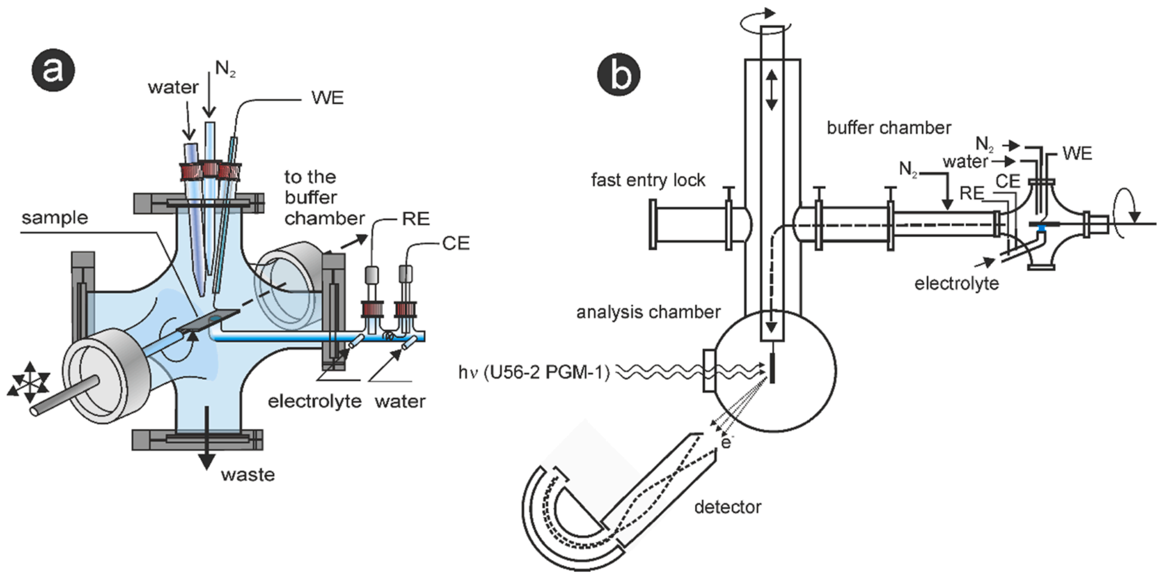

Fig. 1. (a) schematic representation of the in-system SoLiAS electrochemical cell; (b) simplified scheme of the measurement facility.

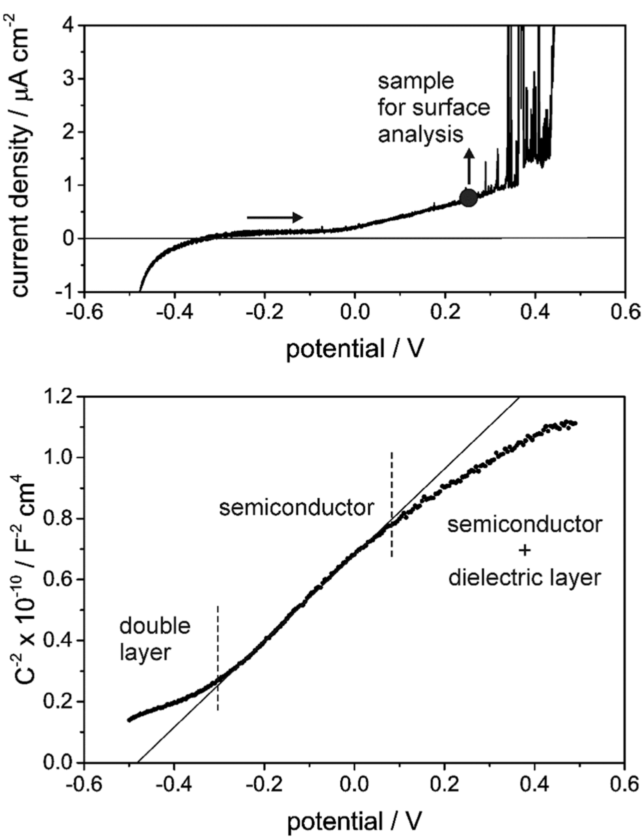

Fig. 2. (a) current-potential curve recorded during the polarization experiment: V_i: − 0.5 V, scan rate: 1 mV s^{-1}; the circle indicates the potential at which the sample was taken out for surface analysis; (b) square of the inverse of capacitance a function of potential measured at 500 Hz.

2. Materials and methods

2.1. Materials

The investigated material consists of steel AISI 309 S, a heat resistant austenitic steel with the composition in at%: Cr 23.7, Fe 61.3, Ni 12.3, C 0.28, Mn 1.15, Si 0.68, P 0.04, S 0.001, Mo 0.13, N 0.1, and Cu 0.19. This composition promotes the formation of 5% of δ-ferrite according to the Schaeffler diagram [20]. Pieces of 6 mm × 6 mm of steel were cut with a water jet cutting machine and polished successively with emery paper up to grit 1000, diamond paste of 6 µm and 1 µm and finally with 0.05 µm alumina suspension. The samples were sonicated in propanol, ethanol, methanol, pure water and finally dried under a nitrogen stream.

An artificial geochemical brine (Q_3) containing 311.57 g/l of NaCl, 2.54 g/l $CaSO_4$, 2.82 g/l K_2SO_4, and 1.95 g/l $MgSO_4$ was used. The solution pH is 5.9. Analytical grade chemicals and ultrapure water (18.2 MΩ·cm Milli-Q system, Millipore) were used for its preparation.

2.2. Methods

The polarization experiment was performed in an electrochemical three electrode cell attached to the synchrotron radiation photoelectron spectroscopy (SR-PES) facility by a buffer chamber (Fig. 1a). The cell was flooded with N_2 during the electrochemical experiment to avoid additional contamination (in-system approach; see Fig.1b). The sample was glued with silver paint on the sample holder and was immediately transferred into the cell. The polished face was brought into contact with the top of L-tube containing the electrolyte until forming a meniscus. Electrochemical measurements were performed by a Solartron electrochemical interface 1287 coupled to a frequency analyzer 1260. A Pt wire and a Ag/AgCl (3 M NaCl) (V_{0ref} = 0.209 V vs NHE) electrode were used as a counter and reference electrodes, respectively. After the potential scan the sample was washed up inside the cell with deaerated Milli-Q water and dried under a N_2 stream. The sample was further transferred to the ultrahigh vacuum (UHV) analysis chamber via the buffer chamber.

The undulator beamline U56–2/PGM-1 at BESSY II (Helmholtz-Centre Berlin) is connected to the dedicated UHV based analysis system SoLiAS (Solid/Liquid Analysis System) end-station equipped with a SPECS Phoibos 150 analyzer based on a delay-line detector. The excitation energy was varied in the range from 100 eV to 1000 eV with an X-ray spot size of 100 µm. This allows tuning the depth of escaping photoelectrons according to their kinetic energy as shown in the appendix. The synchrotron photoelectron spectroscopy system yields typical energy resolutions from 0.010 eV to 0.040 eV in a kinetic energy range of 0–300 eV. The calibration of the binding energy scale was performed at different excitation energies between 100 eV and 1000 eV by measuring the 4 f core level signal of pure Au, set as 84 eV and the corresponding

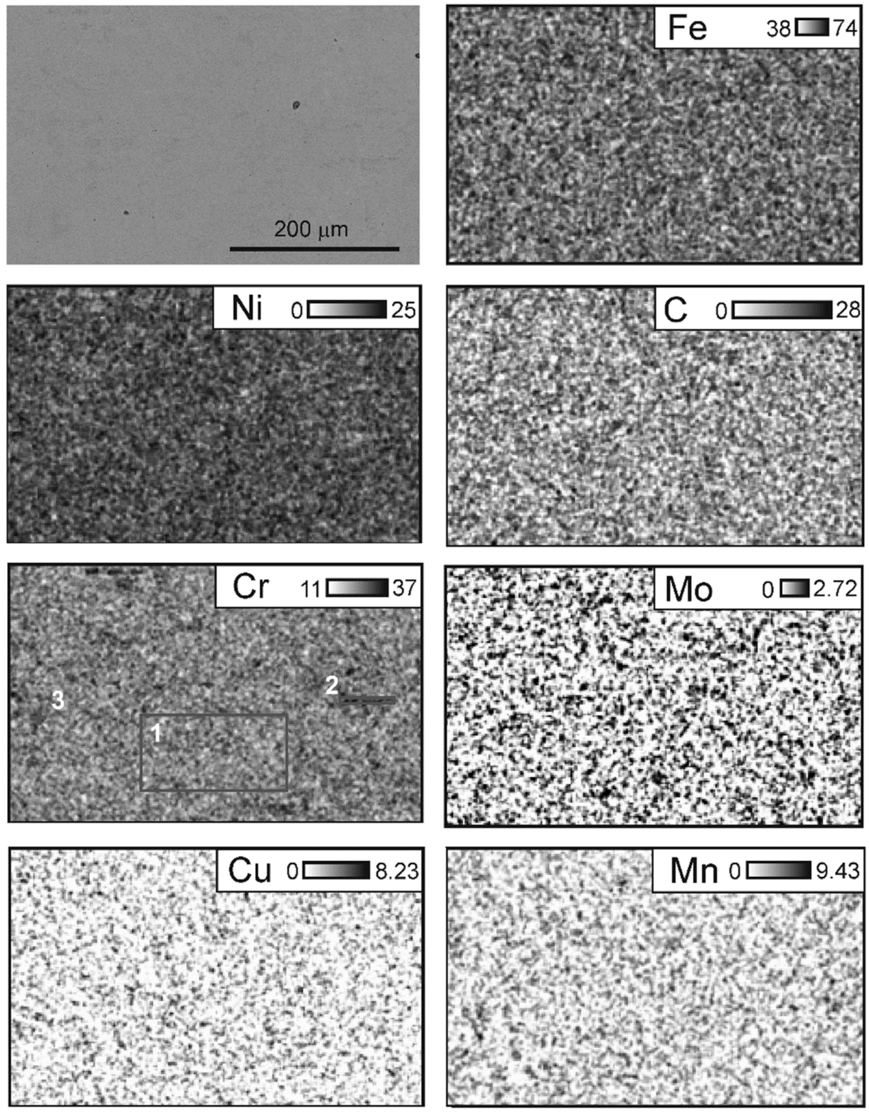

Fig. 3. SEM picture of the 309 S steel surface and corresponding EDX mapping of some selected elements.

Fermi edge.

Electron microscopy was performed with a FEI Quanta 650 FEG scanning electron microscope (now Thermo Fisher Scientific Inc.). SEM-EDX elemental maps were acquired by use of a Thermo Fisher Scientific UltraDry™, i.e., Peltier cooled, silicon drift X-ray detector and analyzed by Pathfinder software version 2.8. The primary electron beam energy was 15 keV.

2.3. Spectra deconvolution

Core-level photoelectron spectra were deconvoluted using the software UNIFIT 2019. The convolution of Lorentzian and Gaussian functions (Voigt profile) was used for the modeling of the peak shapes. The calculation of the background was included in the fitting procedure using a universal background description for inhomogeneous samples. This includes a polynomial component, B_p (E)= $a + b E + c E^2 + d E^3$ which represents the secondary electron background, a Shirley component: $B_S(E) = e S(E)$ and an improved Tougaard background component using a five-parameter inelastic electron scattering cross section: B, C, C′, D and T_0 [21]. In all cases, the calculated background was subtracted after the fitting procedure. The intensity ratio of spin-orbit double peaks and their energy separation were fixed.

3. Results

3.1. Electrochemical studies

Fig. 2a shows the current-potential curve of a potential scan of steel 309 S in Q_3 solution. The scan was run from the cathodic potential limit in the anodic direction after previous stabilization at the open circuit potential during 30 min. The curve indicates a passive behavior until 0.05 V. Next, the current increases almost linearly. Anodic current spikes appear at $E > 0.15$ V, the frequency and height of which increase considerably over 0.35 V. In a second experiment, the surface impedance was measured at 500 Hz following the procedure as in the first run. At this frequency, the system exhibits a predominant capacitive behavior. The interfacial capacitance was calculated assuming a parallel RC-circuit behavior in the whole potential region. Fig. 2b shows the inverse of the square of capacitance as a function of potential (Mott-Schottky plot). Three potential regions can be distinguished. At $E <$ 0.3 V, the curve increases slightly, indicating a double layer control. Between 0.3 V and 0.1 V, an n-type semiconductor behavior dominates. The curve follows a linear relationship according to the Mott-Schottky equation:

$$C^{-2}\ [F^{-2}\ cm^{4}] = (1 / \varepsilon\ \varepsilon_0\ e\ N_D)\ [E - E_{fb} - 0{\cdot}0257] \quad (1)$$

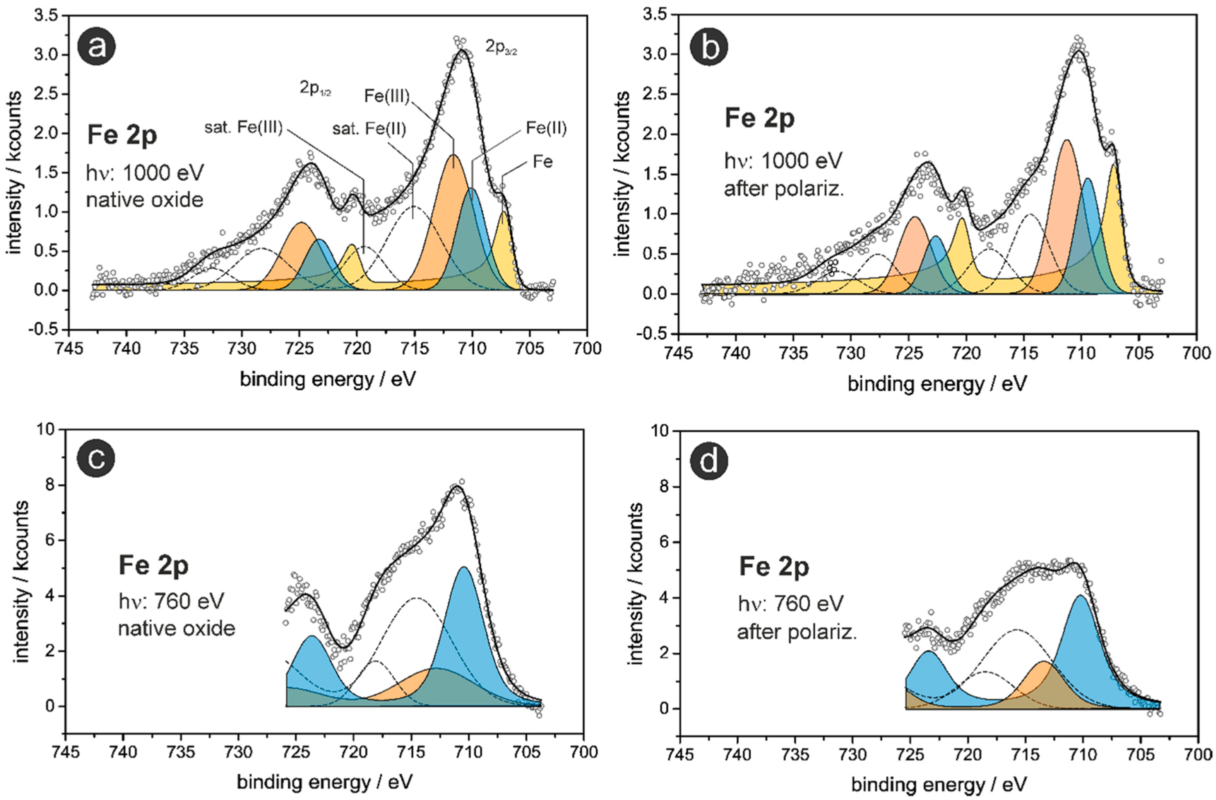

Fig. 4. Fe 2p core level spectra measured before (a) and after the polarization experiment (b) at an excitation energy of 1000 eV; (c) and (d) id. at an excitation energy of 760 eV.

Table 1
Reference binding energies of Fe $2p_{3/2}$ lines.

Fe 2 $p_{3/2}$	E_B / eV	ref.	Fe 2 $p_{3/2}$	E_B / eV	ref.
FeO	709.8 ± 0.5	[27]	$FeCr_2O_4$	710.5	[27]
$Fe_{1.1}O$	709.5 ± 0.2	[26]	FeOOH	711.4 ± 0.4	[27]
Fe_3O_4	710.7 ± 0.4	[27]	α-FeOOH	711.4 ± 0.2	[26]
	709.0 ± 0.2 (2 +)	[26]	γ-FeOOH	711.5 ± 0.2	
	711.4 ± 0.2 (3 +)		$FeCl_2$	710.8 ± 0.3	[27]
Fe_2O_3	711.0 ± 0.4	[27]		710.6 ± 0.2	[26]
α-Fe_2O_3	710.8 ± 0.2	[26]	$FeCl_3$	711.5 ± 0.3	[27]
γ-Fe_2O_3	711.0 ± 0.2			711.5 ± 0.2	[26]
FeOOH	711.4 ± 0.4	[27]	$FeSO_4$	711.0 ± 0.2	[26]
α-FeOOH	711.4 ± 0.2	[26]			

E_{fb} [V] is the flat band potential, ε is the permittivity of the oxide and N_D [cm^{-3}] is the donor density. A density of $N_D = 6.6 \times 10^{20}$ cm^{-3} and a $E_{fb} =$ 0.5 V can be calculated from the slope of the linear part of the curve and the extrapolation to $C^{-2} = 0$, respectively (see Fig. 2b). A permittivity ε = 15.6, reported for the native oxide on stainless steel [22], was adopted. At potentials E > 0.1 V, a dielectric contribution to the interfacial potential drop is indicated by the deviation of the curve from the linear course. On comparing the capacitance- and current-potential curves, it follows that the passive current starts to increase as the n-type semiconductor enters the deep depletion region. SEM-EDX and SR-PES analyses were carried out on a new sample after having stopped the potential scan at 0.25 V (indicated with a circle), just at the beginning of the metastable pitting potential region.

3.2. SEM-EDX analysis

Fig. 3 shows a SEM picture (Z-contrast) and the EDX-mappings of the most relevant alloy elements after the polarization experiment. The surface morphology is homogeneous and only some few pits of 5–10 μm can be observed. The mappings show a relative lateral fluctuation, revealing micro-inhomogeneities of the metallographic steel structure. The quantification performed in the large area 1 (see square in Cr-mapping) yields values similar for the nominal alloy composition: 25.1 at% Cr, 62.3 at% Fe, 12.5 at% Ni and 0.1 at% Mo (in a Cr-Fe-Ni-Mo basis). The analysis at the marked position 2 yields 30%at Cr, 61.3 at% Fe, and 8.2 at% Ni. At point 3, 37 at% Cr and 63 at% Fe. Phases with high Cr content can be assigned to segregated δ-ferrite [23]. It is interesting to note, that minor alloying elements Cu, Mo, Mn, and C, for instance, form evenly distributed clumps, denoting micro-segregation.

3.3. SR-PES measurements

Fig. 4a and b show the Fe 2p core level spectra obtained with an excitation energy of 1000 eV before and after the potential scan, respectively. Only the spin-orbit splitting was considered for the deconvolution of the spectra. It is assumed that the omission of the multiplet splitting [24] caused by crystal-field effects does not affect the precision of the identification of the chemical environment considerably [25]. An acceptable reproduction of the spectra is achieved by introducing five lines. The $2p_{3/2}$ line at 707.30 eV with an asymmetry parameter of 0.3 in the Doniach-Sunjic function can be assigned to metallic iron. The broad lines at 710.08 eV and 711.61 eV can be assigned to Fe^{II} and Fe^{III} respectively (see Table 1). The lines at 715.12 eV and 719.35 eV corresponds to the satellite lines for Fe^{II} and Fe^{III} respectively. A precise identification of the chemical environments seems to be difficult in view of the very close binding energy (BE) of lines of the reference compounds as shown in Table 1. Grosvenor et al. [27] proposed an identification method based on the fine structure of reference oxides (spin-orbit and crystal-field splitting). This method of analysis, however, cannot be straightforwardly applied to disordered oxides due to the lack of knowledge of changes of crystal-field effects with disorder.

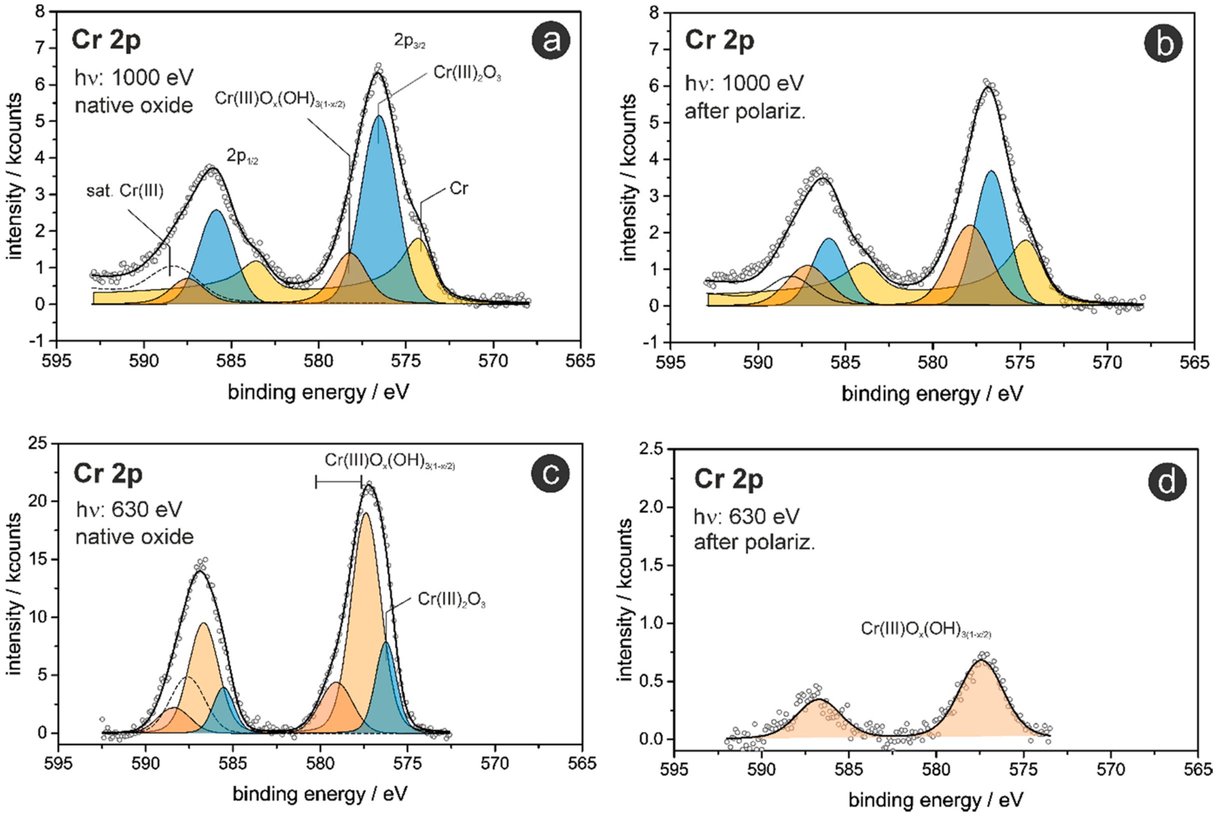

Fig. 5. Cr 2p core level spectra measured before (a) and after the polarization experiment (b) at an excitation energy of 1000 eV; (c) and (d) id. at an excitation energy of 630 eV.

Table 2
Reference binding energies of Cr $2p^{3/2}$ lines.

Cr 2 $p_{3/2}$	E_B / eV	ref.	Cr $2p_{3/2}$	E_B / eV	ref.
CrO_3	579.2 ± 0.6	[26]	$Cr_2(SO_4)_3 \cdot x\ H_2O$	578.5	[30]
Cr_2O_3	576.7 ± 0.2	[26]	$Cr(OH)_3$ (hydrated)	577.3	[30]
$CrCl_3$	577.6 ± 0.2	[26]	Cr_2O_3 (eskolaite)	576.9	[30]
		[30]	$FeCr_2O_4$ (chromite)	576.7	[30]
$NiCr_2O_4$	576.2	[30]	Fe_2CrO_4	576.4	[26]
CrO_2	575.4	[26]			

Fig. 4c and d show surface sensitive spectra obtained with an excitation energy of 760 eV before and after the potential scan, respectively. Their deconvolution was made following the same scheme as before, excluding the metallic line. The high intensity of the synchrotron excitation beam generates an intense emission of secondary electrons, which makes the separation of the dominating background from the core signal very difficult, especially at the lowest values of kinetic energy of photoemitted electrons (see supplemental material). Thus, a cutting of part of the spectra was necessary to facilitate the fitting process.

The spectra are characterized by a predominance of the Fe^{II} lines and their satellites. A shift of the BE of Fe^{II} and Fe^{III} lines by + 0.45 eV and + 1.2 eV respectively is also observed. This effect in commonly observed for surface atoms due to a decrease of coordination (see ref. [27] and citations therein).

Fig. 5a and b show the Cr 2p core level spectra at an excitation energy of 1000 eV before and after the potential scan, respectively. They were deconvoluted in three lines and a Cr^{III} shake-up satellite at 588.3 eV [28, 29] ($2p_{3/2}$). The asymmetric $2p_{3/2}$ line at 574.32 eV can be assigned to chromium metal. The line at 576.55 eV can be assigned to chemical environments found in Cr_2O_3, $FeCr_2O_4$ or Fe_2CrO_4. The line at 578.17 eV indicates a chromium oxyhydroxide (see Table 2).

After the potential scan, the decrease of the intensities of chromium oxide lines is accompanied by an increase of the oxyhydroxide line and of the metallic signal (Fig. 5b).

The surface sensitive spectrum of the native oxide (Fig. 5c) is characterized by a reduction of the chromium oxide signal and a predominance of oxyhydroxide signals at 577.40 eV and 579.08 eV. The latter signal can be attributed to undercoordinated cations at the surface. Fig. 5d shows that the potential scan causes a significant reduction of the signal intensity in the surface sensitive spectrum with a consequent increase of signal noise. The spectrum could be resolved in only one line at 577.40 eV ($2p_{3/2}$).

The mean composition of the native oxide formed on steel 309 S after wet polishing was calculated from the intensities of the oxide lines in the respective core level spectra at an excitation energy of 1000 eV as shown in the appendix. The practical effective attenuation length was calculated taking chromium oxide as a reference (see appendix and Fig. A1). This calculation yields 56.7%at Cr and 43.3%at Fe (in an Fe-Cr basis). The calculated composition remains approximately the same after the potential scan.

Fig. 6a and b show the Cr 3 s signals obtained with a surface sensitive excitation energy of 100 eV before and after the electrochemical polarization, respectively. The deconvolution of the spectrum measured on the native oxide yields two lines: at 75.0 eV and 74.2 eV. The former can be assigned to Cr-OH bonds (as found in the standard spectrum of Cr $(OH)_3$) [30]. The latter is very close to the reported 3 s line for Cr [26], but also for mixed $Fe_{1.4}Cr_{1.6}O_4$ oxide [26]. The assignment to this latter seems more reasonable since low energy photoelectrons are unable to overcome the oxide film. No satellite can be observed at 79 eV as in the standard spectrum obtained with an Al Kα excitation source [30]. This can be ascribed to the large scattering of low energetic photoelectrons. After the polarization, two lines at 77.4 eV and 76.2 eV appears instead of that at 74.2 eV. Standard spectra reported in ref. [30] for $CrCl_3$ indicates a Cr 3 s main peak at 76.6 eV. The peak at 77.4 eV can a priori be ascribed to Cr-OSO_3 bonds. Although no Cr 3 s standard for chromium

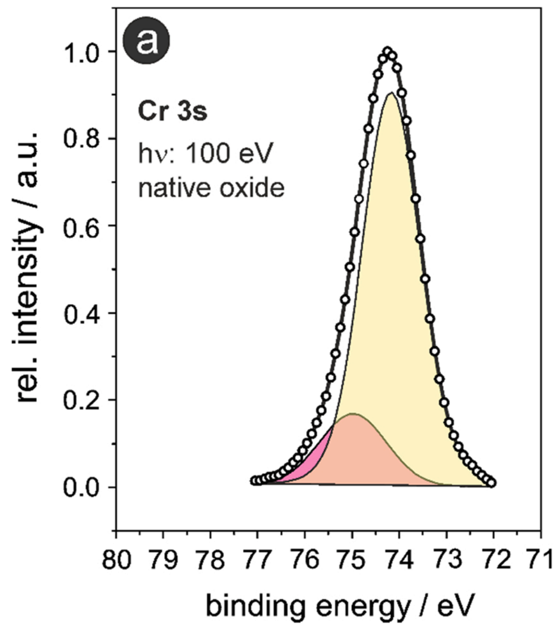

Fig. 6. Cr 3 s core level spectra measured before (a) and after the polarization experiment (b) at an excitation energy of 100 eV.

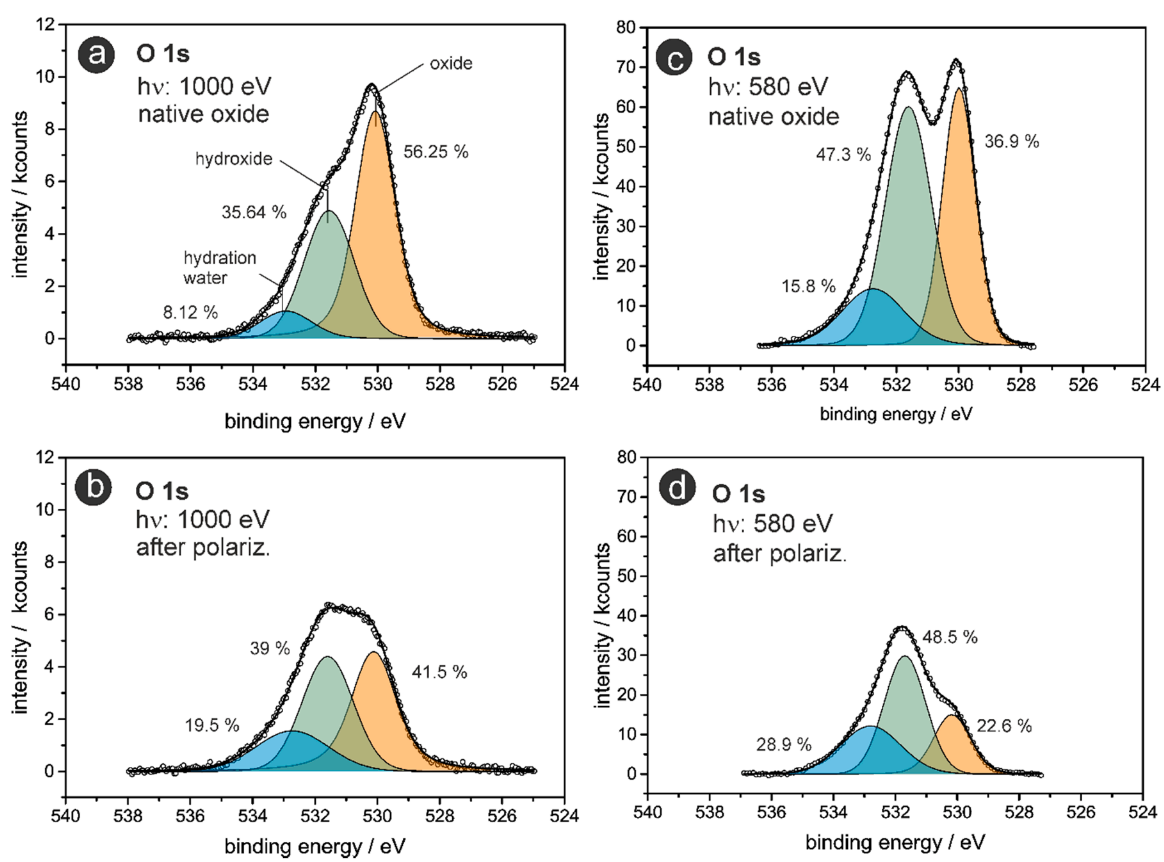

Fig. 7. O 1 s core level spectra measured at an excitation energy of 1000 eV before, (a) and after polarization (c). (b) and (d) id. at an excitation energy of 580 eV.

sulfate could be found in the literature, it is possible to predict this value from the correlation between Cr $2p_{3/2}$ and Cr 3 s BE values reported for other compounds in ref. [26,29,31]. Thus, a value of 77.4 eV can be obtained from this correlation after entering the reported $2p_{3/2}$ value of 578.6 eV for $Cr_2(SO_4)_3{\cdot}15\ H_2O$ [26].

Fig. 7 shows O 1 s spectra obtained at excitation energies of 1000 eV and 580 eV before (a and c) and after (b and d) the potential scan. They could essentially be deconvoluted in three lines: at 530.1 eV, 531.6 eV, and 533.0 eV. According to NIST database [26], the first line can be assigned to M-O bonds (Fe and Cr oxides). The second line can be assigned to M-OH bonds (Fe and Cr oxyhydroxides and hydroxides). The third line can be assigned to OH-groups associated to hydration water

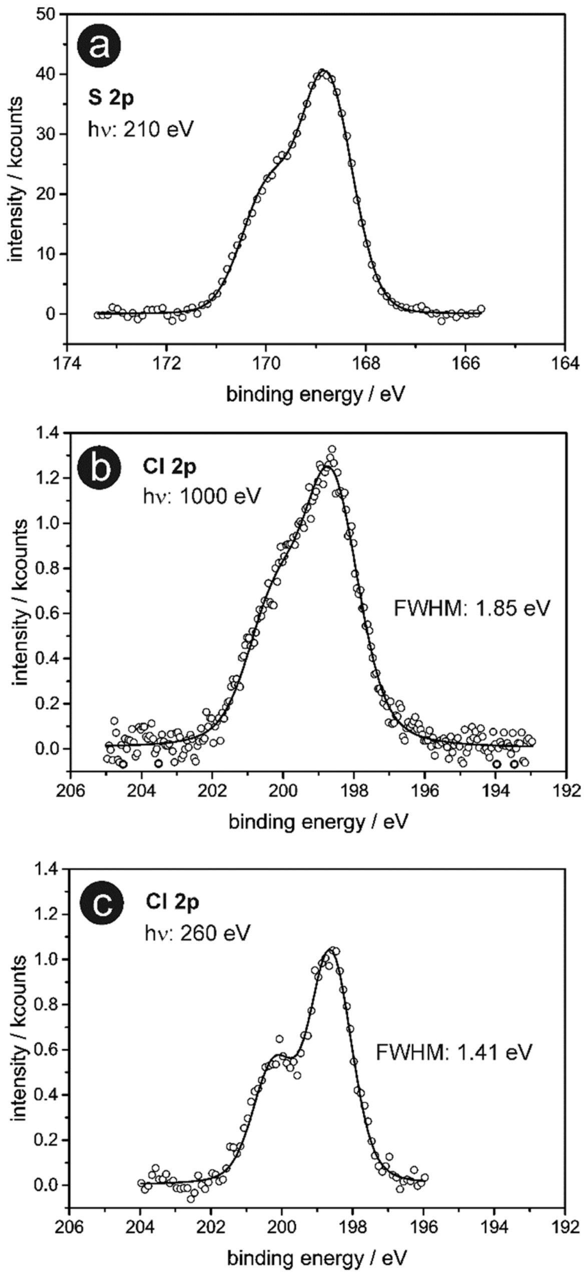

Fig. 8. (a) S 2p core level spectrum measured at hν: 210 eV after polarization; (b) and (c) Cl 2p core level spectra measured at an excitation energy of 1000 eV and 260 eV, respectively, after polarization.

[32]. Signals arising from SiO_2 and O in organic impurities may have some contribution to this line. The former can however be excluded regarding the absence of a definite Si 2p signal. Although a line for the bond C-O is observed in the C 1 s spectrum (see supplemental material), the corresponding contribution to the O 1 s line at 533.0 eV seems to be small, because it does not correlate with the strong decrease observed for C 1 s signal ascribed to adventitious carbon. The integrated line intensities are indicated as % in the figure. Comparing Figs. 7a and 7c, it is seen, that the proportion of hydration water and hydroxyl bonds increases close to the surface in the native oxide. After the polarization, the proportion of hydration water increases together with a reduction of the oxide signal (Fig. 7b). The amount of hydroxyl bonds, however, remains practically the same. A similar, but more marked effect is indicated by the surface sensitive spectrum at 580 eV of excitation.

Fig. 8a shows the surface sensitive S 2p spectrum after the polarization experiment. The S $2p_{3/2}$ line at 168.8 eV can be assigned to SO_4 groups bounded to the oxide. The identification of SO_4 from the O 1 s core level spectrum is somehow difficult, as the BE-region where this line should appear, i.e. 532.3 eV, is dominated by the hydroxyl line.

The Cl 2p spectra at excitations of 1000 eV and 260 eV shown in Fig. 8b and c, respectively could be deconvoluted in only one line at 198.6 eV ($2p_{3/2}$) with different values of the FWHM. The assignment of these lines to definite chemical environments is difficult because of the small energy difference of the $2p_{3/2}$ BE of different metal chlorides. The larger disorder indicated by higher FWHM value at an excitation energy of 1000 eV can be assimilated to different types of M-Cl bonds formed at the inner and outer part of the film.

Fig. 9a and b show low-BE spectra obtained before and after the potential scan at an excitation energy of 100 eV (surface sensitive). Apart from the already analyzed Cr 3 s and O 2 s signals, Fe 3p and Cr 3p signals at 55.54 eV and 43.59 eV respectively, can be identified before the polarization. The Fe3p signal vanishes after the electrochemical experiment, reflecting the release of iron from the outermost part of the film.

Fig. 10a and b show the low BE part of the surface sensitive valence band (VB) spectra at an excitation energy of 100 eV before and after the electrochemical polarization, respectively. They are contrasted with reported valence band spectra of pure chromium and iron oxides [33–35]. The structure of the spectrum of the native oxide at 100 eV presents characteristic features at 2.7 eV (A), 5.4 eV (B), 10.1 eV (C), and 13.6 eV (D) which can be associated to those appearing in the reference spectra.

After the potential scan, the intensity of the VB spectrum drops by one order of magnitude. There is also a shift of the feature B by + 0.85 eV (B) and a decrease of the relative intensity of feature A by ca. 25%. The spectrum approaches that reported for $Cr(OH)_3{\cdot}0.4\ H_2O$.

Fig. 10c and d show the rising part of the VB spectra at 100 eV excitation near the Fermi level. The spectra present a linear course between 1.2 eV and 2 eV. Their extrapolation to zero indicates the position of the semiconductor valence band by 0.7 eV and 0.8 eV below the Fermi level before and after the electrochemical experiment, respectively. The intensity of the tail between 1.0 eV and 0.5 eV denotes the presence of a large number of interfacial states, as typical for disordered surfaces.

4. Discussion

The 2p core level spectra of Fe and Cr indicate that a mixed oxide constituted by Fe^{II}, Fe^{III} and Cr^{III} species forms on stainless steel 309 S after wet polishing. An identification of the chemical environments based on reference spectra only seems to be impracticable (Figs. 4 and 5). This is due to (i) the relative line widening introduced by the disordered oxide structure (FWHM between 2 and 3 eV) and (ii) the variety of chemical environments expected in a mixed oxide.

The surface sensitive Fe 2p core level spectra (Fig. 4c) indicate a significant increase of disorder and a predominance of Fe^{II} at the surface. The corresponding surface sensitive Cr 2p core level spectrum (Fig. 5c) indicates a preponderance of hydrated chromium oxide, represented by lines at 577.4 eV and 579.13 eV.

The large intensities of the lines attributable to hydration water in the deconvoluted bulk and surface sensitive O 1 s core level spectra (Fig. 7) points out a highly hydrated native oxide. An interesting aspect of these spectra is the increase of the signal referring to M-OH bounds close to the oxide surface. This result would be in line with the predominance of $Cr(OH)_3$ and FeOOH at the outmost part of a mixed iron-chromium oxide layer proposed by others [5,6].

The Fe^{II} lines in the Fe 2p spectra can be ascribed to Fe-OH bonds as these lines are linked up with larger Fe^{II} satellite lines. The reference spectra of Fe^{II}-oxides and -halides [27] show that the satellite signals of these latter are significantly larger than those of oxides. The effect is attributed to a decrease of the electronegativity of the anion [36].

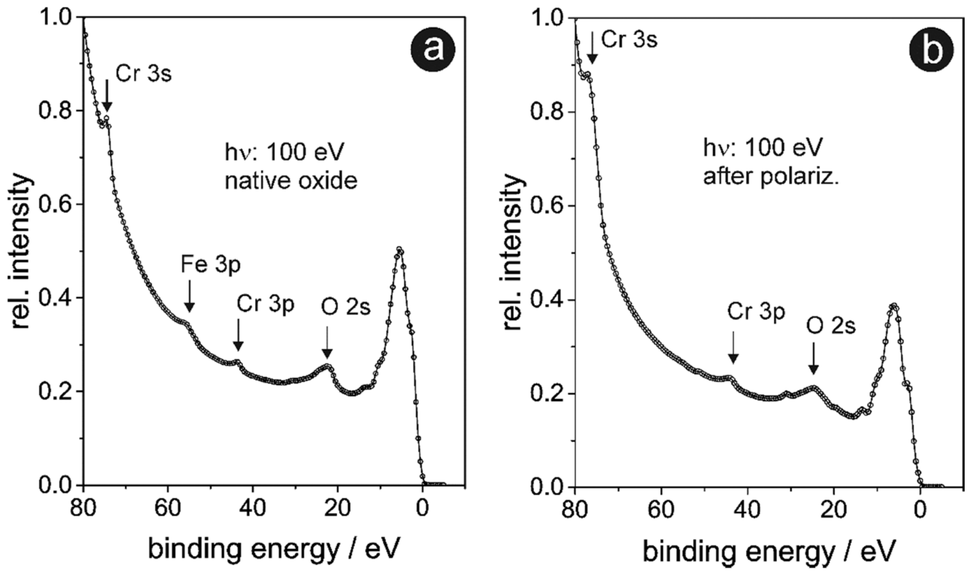

Fig. 9. Low binding energy spectra measured at an excitation energy of 100 eV before (a) and after (b) the polarization experiment.

Despite the lack of deconvoluted reference data for iron hydroxide, an analogy of chloride and OH^- seems feasible. Therefore, the increase of the satellite line in the surface sensitive spectra would indicate an increase of the OH^-/O^{2-} ratio upon hydroxylation of the outermost part of the oxide.

The ratio Fe^{III}/Fe^{II} in the native oxide is about 1.77, whereas the ratio O^{2-}/OH^- is 1.23. Thus, an average formula $FeCr_{1.54}O_{2.58}OH_{2.1}$ for the native oxide can be calculated from the charge neutrality. This composition can be analogized to a hydrated [x Cr_2O_3 + (1-x) Fe_3O_4] oxide, where the hydration extent increases towards the surface.

Using this formula, an oxide thickness of about 2.3 nm can be calculated from the intensity ratios (I_{metal}/I_{oxide}) for iron and chromium following the method described in the appendix. A density of 4.2 g cm^{-3} was adopted for the mixed oxyhydroxide (a mean value of those reported for FeOOH: 4.25, CrOOH: 4.13 [37]). The thickness values calculated from Fe 2p and Cr 2p spectra (Figs. 4a and 5a) equal for a surface metal composition of $X_{Cr} = 0.44$.

The anodic polarization causes an increase of the metal signal by a factor of 1.67 and a reduction of the FWHM of the oxide lines (Fig. 4a and b). This latter is also observed for the surface sensitive spectra (Fig. 4c and d). The change can be interpreted as a preferential dissolution of iron at the more defective surface oxide structure. The Cr 2p core level spectra at 1000 eV of excitation energy show an increase of hydroxide/oxide intensity ratio from 0.29 to 0.77 maintaining the total intensity. This indicates a hydroxylation of a considerable part of the Cr-O bonds.

Particularly notable is the drop of intensity of the surface sensitive Cr 2p core level spectrum by a factor of 10 after polarization. A tentative explanation is based on the formation of an outer sub-nanometer rough, gel-like layer of chromium hydroxide after hydroxylation and partial dissolution of iron which attenuates the emitted photoelectron flux from this overlayer at the detection angle [38]. This effect becomes stronger as the overlayer thickness is larger than the attenuation length, i.e. $\geq$ 0.5 nm (see Fig. A1). The Fe 2p signal measured after the polarization experiment arises mainly from the mixed oxide sublayer under the porous $Cr(OH)_3$, whose intensity is now attenuated. This also explains the low intensity of the surface sensitive spectra shown in Fig. 4c and d.

The selective dissolution process involves the hydroxylation and breakdown of Fe-O-Fe bridges in the mixed hydrated oxide involving water deprotonation (see model discussion below). This explains the marked decrease of the oxide line at 530 eV in the O 1 s spectra (M-O bonds) after the polarization (Fig. 7a and b) and the relative larger concentration of M-OH bonds.

The hypothesis of a selective dissolution of iron at the oxide-electrolyte interface is further supported by the vanishing of the Fe 3p signal from the low-BE spectra shown in Fig. 9. The shape and the features A to D of surface sensitive valence band spectrum of the native oxide (Fig. 10a) can be associated with the reference spectra of hydrated $Cr(OH)_3$ and FeOOH. The similarity of the spectrum with that of hydrated chromium oxide is more marked after the potential scan (Fig. 10b), in line with the presumption of a selective dissolution of iron.

The energy diagrams shown in Fig. 11 represent the electronic aspects of the metal-oxide-electrolyte interface at the start and at the end of polarization, as obtained from the valence band spectra (Fig. 10) and the capacitance-potential curve (Fig. 2). A value of 4.5 eV for the hydrogen standard electrode potential was adopted. The native oxide consists of a n-type semiconductor with a flat band potential at 0.5 V. The metal-oxide interface is assumed in electronic equilibrium. The alignment of Fermi levels is absorbed by a large density of interface states, generating an interfacial dipole ($\Delta\varphi_{dip}$). Secondary electron edge measurements (not shown) let determine the Fermi level of the alloy at 4.2 eV. Thus, regarding the reported value of 5.0 eV for stainless steel [39], the interfacial dipole can be estimated by 0.8 eV. According to the extrapolation of the raising part of the valence band spectrum to zero intensity, the valence band edge of the semiconductor is 0.8 eV below the Fermi level.

The spectroscopic signal attributed to Fe^{II} species in the native oxide is probably related with charged gap states arising from defects, e.g. undercoordinated sites. This would explain the corresponding large satellite signal, associated with Fe^{II}-OH bonds. Undercoordinated sites are expected to stack at the oxide surface. These oxide defects create a large density of gap states near the semiconductor band edges. They introduce energy states reflected by the intensity tail appearing in the low BE part of the VB spectrum between valence band edge (linear extrapolation) and the Fermi level.

As the potential is shifted towards values more positive than 0.2 V, the semiconductor turns in deep depletion and large amounts of holes accumulate at the oxide-electrolyte interface. Parallelly, localized surface states are discharged. This assists the splitting of Cr-O and Fe-O bonds in the outer mixed oxide layer by reacting with water, as exemplified in reaction scheme shown in Fig. 12. The complete hydroxylation of iron results in the formation of soluble species leaving a disordered and open structured $Cr(OH)_3$ film. This layer behaves as a dielectric, capturing a fraction of the interfacial potential drop. Moreover, the

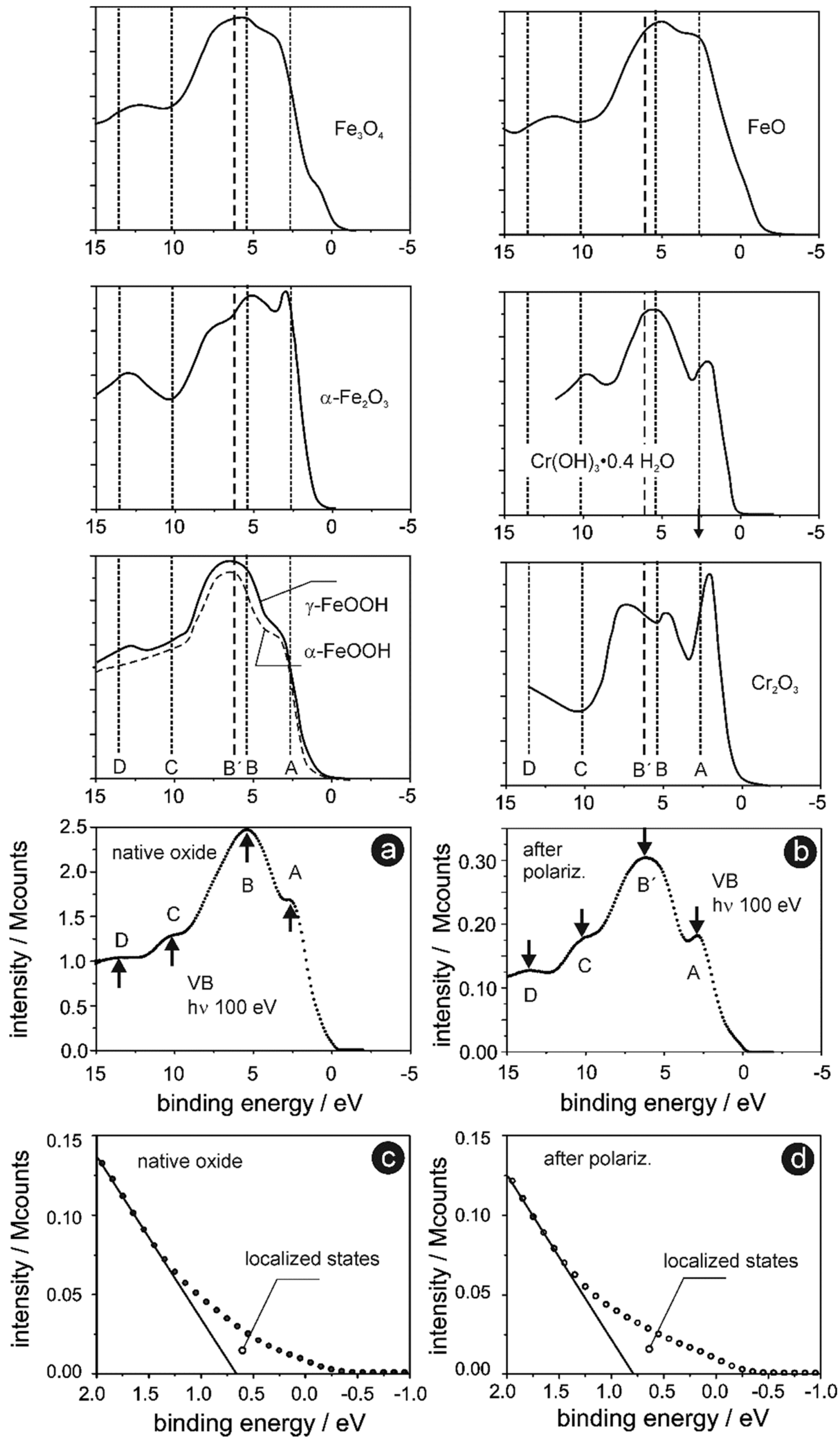

Fig. 10. (a) and (b) valence band spectra measured at an excitation energy of 100 eV before and after the polarization experiment, respectively, contrasted with published reference spectra for various iron and chromium oxides from ref. [33–35]; (c) and (d) rising part of spectra (a) and (b).

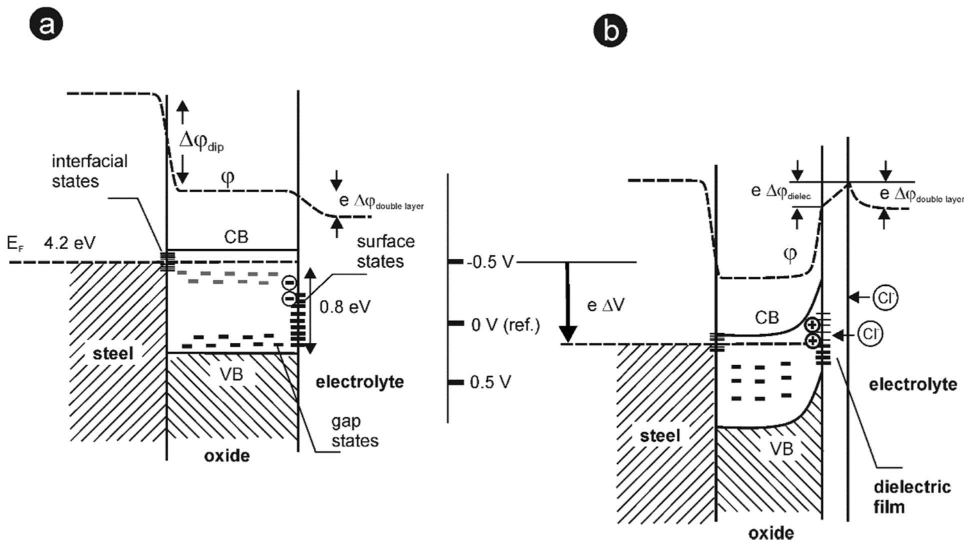

Fig. 11. Energy diagrams of the steel-oxide-electrolyte interface outlined from the spectroscopic and electrochemical data: (a) native oxide at its flat band potential; (b) at 0.2 V.

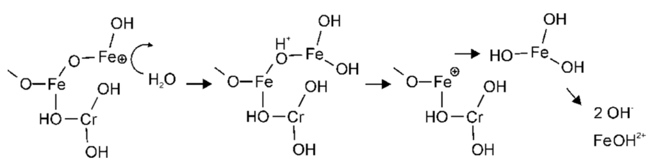

Fig. 12. Reaction mechanism exemplifying the hydroxylation of Fe-O bonds assisted by holes followed by formation of soluble species.

created electric field stimulates the ingress of chloride, thus favoring the dissolution process. The scenario in the pre-pitting potential region is visualized in Fig. 13. The inner part of the oxide is constituted by a Cr-rich iron-chromium oxide which changes over to a mixing of hydrated Fe_3O_4 and $Cr(OH)_3$ at the outermost part of the layer. The thickness of the native oxide equals ca. 8–12 at. layers. The release of iron ions from the oxide network leaves sub-nanometer spaces allowing the access of water and chloride ions, which in turn accelerates the growth of cavities. Moreover, the n-type semiconduction of the oxide is an evidence of oxygen vacancies [40]. They can be considered as an additional a path for penetration of chloride towards the metal-oxide interface.

The formation of Cr-Cl and Cr-OSO_3 bonds was evidenced by the surface sensitive Cr 3 s spectra (Fig. 6). The low excitation energy and the consequent low kinetic energy of photoelectrons yield intensive signals arising from one or two surface monolayers with a low intensity of secondary electrons. Moreover, the absence of multiplet-splitting allows a more precise assignment. The identification of Cr-Cl and Cr-OSO_3 bounds in surface sensitive Cr 2p core level spectrum is not unambiguous because of large intensity of secondary electrons yielding a low signal-to-noise ratio.

The larger FWHM of the Cl 2p line at an excitation energy of 1000 eV than that measured at 260 eV suggests whether a larger disorder of M-Cl bonds or the overlap of different types of metal-chloride bonds inside the oxide layer. It must be noted, that the intensity of the Cl 2p line at

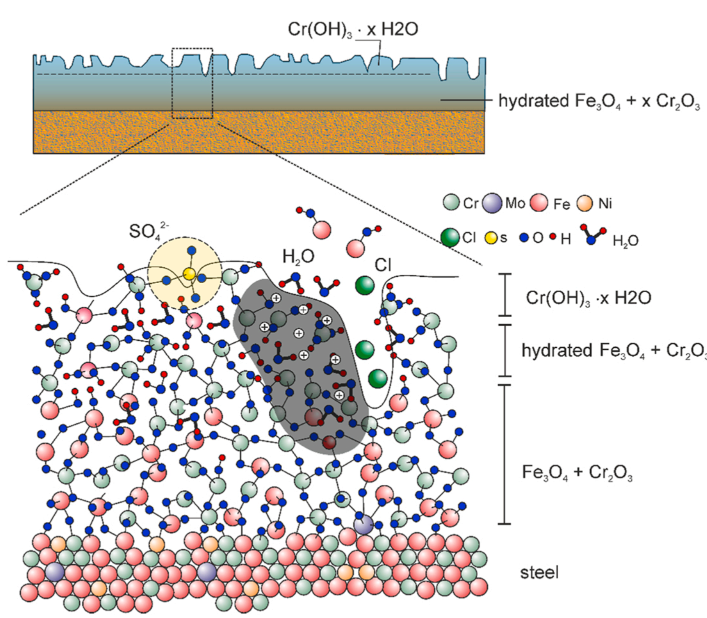

Fig. 13. Steel-oxide interface depicting the formation of nanoscale cavities by selective dissolution the iron in the mixed oxy-hydroxide and a representative atomic structure.

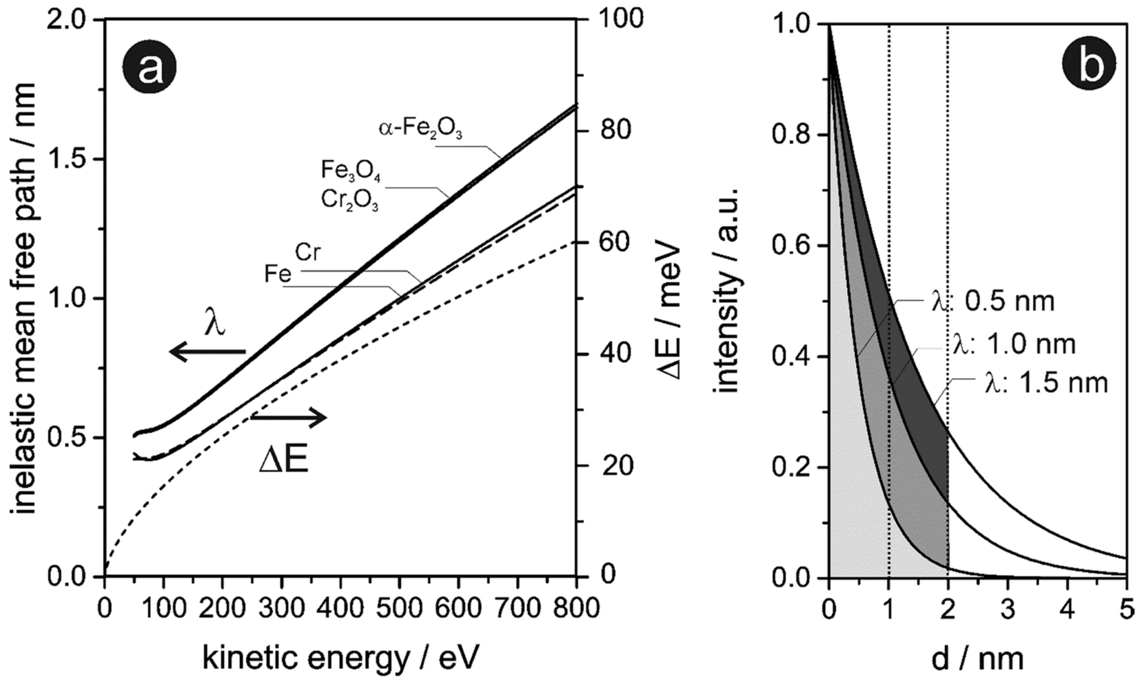

Fig. A1. (a) Inelastic mean free path (IMFP) for various metals and oxides and typical binding energy resolution of a synchrotron photoelectron spectroscopy facility as a function of the kinetic energy of photoelectrons; (b) photoelectron flux as a function of the excitation depth calculated for different values of the IMFP.

260 eV of excitation is in the same order of magnitude as that observed for 1000 eV spite of 30-fold larger photoionization cross section of former. This result is in line with the signal attenuation introduced by a sub-nanometer rough overlayer. At this stage, it is not possible to ensure, that there is a penetration of chloride into the oxide. Natishan et al. [41] found that below the pitting potential of 316 L steels, chloride is incorporated in the oxide only when it grows in the chloride solution. Therefore, it appears that the Cl 2p signal for large values of the electron free path reflects the chemistry of inward growing channels created by formation of metal-chloride bonds during the progressive hydration. The presence of sulfate in a concentration of 0.05 mol l^{-1} exerts a significant influence on the passivation behavior as shown in ref. [23]. Inasmuch as sulfate was detected only at the surface oxide, it is probably that sulfate ions block the penetration of chloride by bridging adjacent hydroxylated bonds.

5. Conclusions

A comprehensive study of the compositional and structural transformations of the native oxide film on stainless steel 309 S during the anodic polarization prior to the onset of pitting in high saline synthetic geological brine was carried out by applying synchrotron x-ray photoelectron spectroscopy. Initially, the native oxide formed during wet polishing consisted of a thin disordered, highly hydrated Cr-rich oxide which can be modelled by a layer akin to a mixed $Fe_3O_4 + Cr_2O_3$ which is strong hydrated towards the surface. The film behaves as a highly dopped n-type semiconductor which is in accumulation near the pitting potential. The discharge of localized states drives the hydroxylation of M-O-M (M: Cr, Fe) bridges in the oxide by reaction with water. This leads to the release of iron by formation of soluble products. The selective dissolution of iron and the strong oxide hydration leaves a surface hydrated $Cr(OH)_3$ with an open structure which facilitates the inward migration of chloride, also driven by the surface positive charge during the anodic polarization. Sulfate ions probably counteract the dissolution process by closing the broken structure.

CrediT authorship contribution statement

Andrés G. Muñoz: Conceptualization, Investigation, Methodology, Writing – original draft, Resources, Funding acquisition, Writing – review & editing **Thorsten Mayer**: Investigation **Dieter Schild**: Investigation, Data curation, Resources, Writing – review & editing **Wolfram Calvet**: Investigation, Supervision, Resources.

Declaration of Competing 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.

Data Availability

Data will be made available on request.

Acknowledgements

The Federal Ministry for Economic Affairs and Energy (BMWi) is gratefully acknowledged for the funding of this work (contract number 02 E11496).

Appendix

Synchrotron-radiation photoelectron spectroscopy facility

The synchrotron radiation facility let vary the kinetic energy of emitted photoelectrons by setting the beam energy between 100 and 1000 eV. As the inelastic mean free path (IMFP) of photoelectrons increases with the kinetic energy as shown in Fig. A1 for Fe and Cr and their oxides, the excitation depth can be changed from a couple of atomic layers so some nm. Fig. A1b shows the characteristic exponential decay of the photoelectron flux with depth for different values of the IMFP. The synchrotron facility also yields a high energy resolution typically from 10 meV to 40 meV depending on the kinetic energy [42].

Composition of the film

The elementary concentration of the film was calculated using the expression:

$$\%\text{at } i = \{I_{i\ (ox)} / [\sigma_{i,h\nu}\ \lambda_{i,ox}(E_i)\ T(E_i)]\} / \Sigma_i\ \{I_{i\ (ox)} / [\sigma_{i,h\nu}\ \lambda_{i,ox}(E_i)\ T(E_i)]\} \tag{A.1}$$

where i: Fe, Cr, $I_{i\ (ox)}$ is the integral intensity of the oxide lines for the element i, $\sigma_{i,h\nu}$ is the photoionization cross section of the element i at the corresponding core level for an excitation hν, $\lambda_{i,ox}(E_i)$ is the practical effective attenuation length in the oxide for the element i at the kinetic energy E_i. This value depends on the asymmetry factor of the corresponding element and on the incidence angle. They were calculated using the NIST Electron Effective-Attenuation-Length Database [43]. Values of $\sigma_{i,h\nu}$ were taken from ref. [44]. $T(E_i)$ is the transmission function of the analyzer, which was assumed to be constant.

Oxide thickness calculation

The thicknesses of the oxide covering the alloy can be calculated from the relations of metal to oxide intensity of the core level spectra of Cr and Fe. The intensity of the oxide line for a given element is given:

$$I_{i\ (ox)} = I^0_{i\ (ox)}\ \{1\text{-exp}[\text{-}d_{ox}/\lambda_{ox}(E_i)\ \cos\theta]\} \tag{A.2}$$

The signal from the alloy can be expressed as:

$$I_{i\ (m)} = I^0_{i\ (m)}\ \exp[\text{-}d_{ox}/\lambda_{ox}(E_i)\ \cos\theta] \tag{A.3}$$

$I_{i\ (ox)}$ is the total intensity of the element *i* in the oxide. $I^0_{i\ (ox)}$ and $I^0_{i\ (m)}$ are the reference intensities of a pure oxide and of the alloy (m: matrix) respectively. $\lambda_{ox}(E_i)$ is the inelastic mean-free-path of excited electrons in the oxide at the kinetic energy E_i. θ is the electron emission angle: π/4. From of Eq.(A.2)–(A.3), the following expressions for d_{ox} can be derived:

$$d_{ox} = \ln\ [(I_{i\ (ox)}/I_{i\ (m)}) \times (I^0_{i\ (m)}/I^0_{i\ (ox)}) + 1] \times \lambda_{ox}\ (E_i) \tag{A.4}$$

The inelastic mean free path in the oxides was calculated using the Tanuma-Powel-Penn equation (see ref.[38]).
The relation $(I^0_{i\ (ox)}/I^0_{i\ (m)})$ was calculated by the relation:

$$(I^0_{i\ (m)}/I^0_{i\ (ox)}) = X_i \times N^0_{av} \times \lambda_{av}(E_i) \times P_{i\ (m)}/\ [N^0_{ox} \times \lambda_{\ ox}\ (E_i)] \tag{A.5}$$

where X_i is the atomic fraction of the metal *i* in the alloy, N^0_{ox} is the density of atoms of element i in the oxide. $P_{i\ (m)}$ is a weak matrix correction assumed near unity. N^0_{av} is the atom density of the average matrix concept (alloy) as proposed by Seah and Gilmore (see ref.[38]; 5.20×10^{22} cm^{-3}. $\lambda_{av}(E_i)$ is the corresponding energy dependent inelastic mean free path:

$$\lambda_{av}(E)\ [\text{nm}] = 0{\cdot}000523\ E^3 / [\ 48{\cdot}6 - 1{\cdot}76\ E + 0{\cdot}518\ E^2\ (\ln E\text{-}2{\cdot}61)] \tag{A.6}$$

See Appendix Fig. A1.
The raw/processed data required to reproduce these findings cannot be shared at this time due to technical or time limitations.

References

[1] T. von Berlepsch, B. Haverkamp, Salt as a rock for the geological repository for nuclear waste, Elements 12 (2016) 257–262.
[2] T. von Berlepsch, Salt repository systems: Design development approach at the example of the Gorleben salt dome, in: M.J. Apted, J. Ahn (Eds.), Geological repository systems for safe disposal of spent nuclear fuels and radioactive waste, Ch.6, Woodhead Publishing Series in Energy, Elsevier, 2017, pp. 145–162.
[3] T. Hassel, A. Köhler, Ö.S. Kurt, Das ENCON-Behälterkonzept – Generische Behältermodelle zur Einlagerung radioaktiver Reststoffe für den interdisziplinären Optionenvergleich, ENTRIA-Arbeitsbericht-16. Hannover, Leibniz University Hannover, 2019.
[4] F. King, M. Kolář, P.G. Keech, Simulations of long-term anaerobic corrosion of carbon steel containers in Canadian deep geological repository, Corr. Eng. Sci. Tech. 49 (2014) 455–459.
[5] L. Wang, A. Seyeux, P. Marcus, Ion transport mechanisms in the oxide film formed on 316L stainless steel surfaces studied by ToF-SIMS with $^{18}O_2$ isotopic tracer, J. Electrochem. Soc. 167 (2020), 101511.
[6] Z. Wang, A. Seyeux, S. Zanna, V. Maurice, P. Marcus, Chloride-induced alterations of the passive film on 316L stainless steel and blocking effect of pre-passivation, Electrochim. Acta 329 (2020), 135159.
[7] L. Olefjord, B. Brox, U. Jelvestam, Surface composition of stainless steels during anodic dissolution and passivation sudied by ESCA, J. Electrochem. Soc. 132 (1985) 2854.
[8] C. Leygraf, G. Hultquist, I. Olefjord, B.-O. Elfström, V.M. Knyazheva, A. V. Plaskeyev, Ya.M. Kolotyrkin, Corros. Sci. 19 (1979) 343–357.
[9] P. Keller, H.-H. Strehblow, XPS investigations of electrochemically formed passive layers on Fe/Cr-alloys in 0.5 M H2SO4, Corros. Sci. 46 (2004) 1939–1952.
[10] S. Tardio, M.-L. Abel, R.H. Carr, J.E. Castle, J.F. Watts, Comparative study of the native oxide on 316L stainless steel by XPS and ToF-SIMS, J. Vac. Sci. Technol. A 33 (2015), 05E122-1-14.
[11] Z. Wang, E.-M. Paschalidou, A. Seyeux, S. Zanna, V. Maurice, P. Marcus, Mechanisms of Cr and Mo enrichments in the passive oxide film on 316L austenitic stainless steel, Front, Mater 6 (2019) 232.
[12] Z. Szklarska-Smialowska, Mechanism of pit nucleation by electrical breakdown of the passive film, Corros. Sci. 44 (2002) 1143–1149.

[13] P.M. Natishan, W.E. OGrady, F.J. Martin, R.J. Rayne, H. Kahn, A.H. Heuer, Chloride interactions with the passive films on stainless steel, J. Electrochem. Soc. 158 (2011) C7–C10.
[14] G.T. Burstein, C. Liu, R.M. Souto, S.P. Vines, Origins of pitting corrosion, Corros. Sci. Tech. 39 (2004) 25–30.
[15] T.P. Hoar, W.R. Jacob, Breakdown of passivity of stainless steel by halide ions, Nature 216 (1967) 1299–1301.
[16] H.H. Strehblow, in: P. Marcus, J. Oudar (Eds.), Corrosion Mechanism in Theory and Practice, Marcel Dekker, New York, 1995, p. 201.
[17] P.C. Pistorius, G.T. Burstein, Aspects of the effects of electrolyte composition on the occurrence of metastable pitting on stainless steel, Corros. Sci. 36 (1994) 525–538.
[18] C.Y. Chao, L.F. Lin, D.D. Macdonald, A point defect model for anodic passive films. II. Chemical breakdown and pit initiation, J. Electrochem. Soc. 128 (1981) 1191–1198.
[19] H.P. Leckie, H.H. Uhlig, Environmental factors affecting the critical potential for pitting in 18-8 stainless steel, J. Electrochem. Soc. 113 (1966) 1262–1267.
[20] S.D. Washko, G. Aggen, Wrought Stainless Steels in ASM Handbook, in: Properties and selection: Irons, steels, and high-performance alloys, Volume 1, ASM International, 1990.
[21] R. Hesse, M. Weiβ, R. Szargan, R. Streubel. R. Denecke, Improved peak-fit procedure for XPS measurements of inhomogeneous samples—Development of the advanced Tougaard background method, J. Electron. Spectrosc. Relat. Phenom. 205 (2015) 29–51.
[22] G. Okamoto, T. Shibata, Stability of passive stainless steel in relation to the potential of passivation treatment, Corros. Sci. 10 (1970) 371–378.
[23] A.G. Muñoz, D. Schild, Corrosion of steel in high-level radioactive waste rock repositOries: Kinetics and thermodynamics, Corros. 2018, Phoenix, Ariz., USA, April (2018). Paper Number: NACE-2018-11707.
[24] R.P. Gupta, S.K. Sen, Calculation of multiplet structure of core p-vacancy levels, II, Phys. Rev. B 12 (1975) 15.
[25] T. Yamashita, P. Hayes, Analysis of XPS spectra of Fe^{2+} and Fe^{3+} ions in oxide materials, Appl. Surf. Sci. 254 (2008) 2441–2449.
[26] NIST X-ray photoelectron spectroscopy database, NIST Standard Reference Database Number 20, 20899, National Institute of Standards and Technology,, Gaithersburg MD, 2000, https://doi.org/10.18434/T4T88K.
[27] A.P. Grosvenor, B.A. Kobe, M.C. Biesinger, N.S. McIntyre, Investigation of multiplet splitting of Fe 2p XPS spectra and bonding in iron compounds, Surf. Interface Anal. 36 (2004) 1564–1574.
[28] A.M. Salvi, J.E. Castle, J.F. Watts, E. Desimoni, Peak fitting of the chromium 2p XPS spectrum, Appl. Surf. Sci. 90 (1995) 333–341.
[29] M. Aronniemi, J. Sainio, J. Lahtinen, Chemical state quantification of iron and chromium oxides using XPS: the effect of the background subtraction method, Surf. Sci. 578 (2005) 108–123.
[30] T. Gross, D. Treu, E. Ünveren, E. Kemnitz, W.E.S. Unger, Characterization of Cr(III) compounds of O, OH, F and Cl by XPS, Surf. Sci. Spect. 15 (2008) 77–123.
[31] T.P. Moffat, R.M. Latanision, An electrochemical and x-ray photoelectron spectroscopy study of the passive state of chromium, J. Electrochem. Soc. 139 (1992) 1869–1878.
[32] H. Sanchez Casalongue, S. Kaya, V. Viswanathan, D.J. Miller, D. Friebel, H. A. Hansen, J.K. Nørskov, A. Nilsson, H. Ogasawara, Direct observation of the oxygenated species during oxygen reduction on a platinum fuel cell cathode, Nat. Commun. 4 (2013) 2817.
[33] W. Temesghen, P.M.A. Sherwood, Analytical utility of valence band X-ray photoelectron spectroscopy of iron and its oxides, with spectral interpretation by cluster and band structure calculations, Anal. Bioanal. Chem. 373 (2002) 601–608.
[34] K. Asami, K. Hashimoto, The X-ray photo-electron spectra of several oxides of iron and chromium, Corros. Sci. 17 (1977) 559–570.
[35] I. Ikemoto, K. Ishii, S. Kinoshita, H. Kuroda, M.A. Alario Franco, J.M. Thomas, X-ray photoelectron spectroscopic studies of CrO_2 and some related chromium compounds, J. Solid State Chem. 17 (1976) 425–430.
[36] D.D. Sarma, P. Vishnu Kamath, C.N.R. Rao, Satellites in the X-ray photoelectron spectra of transition-metal and rare-earth compounds, Chem. Phys. 73 (1983) 71–82.
[37] J.W. Anthony, R.A. Bideaux, K.W. Bladh, M.C. Nichols, Handbook of Mineralogy. Mineralogical Society of America, Chantilly,, VA, USA, 2003.
[38] S. Hoffmann, Auger- and X-ray Photoelectron Spectroscopy in Materials Science, Springer, Heidelberg, 2013, p. 214.
[39] N. Barrett, O. Renault, H. Lemaître, P. Bonnaillie, F. Barcelo, F. Miserque, M. Wang, C. Corbel, Microscopic work function anisotropy and surface chemistry of 316L stainless steel using photoelectron emission microscopy, J. Electron. Spectrosc. Relat. Phenom. 195 (2014) 117–124.
[40] P.A. Cox, Transition Metal Oxides, Clarendon Press, Oxford, 1992 (republished 2010).
[41] P.M. Natishan, W.E. O'Grady, F.J. Martin, R.J. Rayne, H. Kahn, A.H. Heuer, Chloride interactions with the passive films on stainless steel, J. Electrochem. Soc. 158 (2011) C7–C10.
[42] K. Shimada, Hard X-ray valence-band and core-level photoelectron spectroscopy of strongly correlated electron systems, Nucl. Instrum. Methods Phys. Res. A 547 (2005) 169–175.
[43] C.J. Powell, A. Jablonski, NIST Standard Reference Database 82. NIST Electron Effective-Attenuation-Length Database. Version 1.3, NIST, 2011 (Maryland).
[44] J.J. Yeh, I. Lindau, Atomic subshell photoionization cross sections and asymmetry parameters: $1 \leq Z \leq 103$, . Data Nucl. Data Tables 32 (1985) 1–155.

Deconvolution of Fe 2p and Cr 2p core level spectra

The deconvolution of Fe 2p core level spectra at an excitation energy of 1000 eV was made by assuming lines corresponding to metal, Fe(II), Fe(III) and the corresponding satellite lines. The background was included in the fitting procedure using a universal expression as explained in the section materials and method of the present article. This procedure is especially appropriate for the surface sensitive spectra performed at an excitation energy of 760 eV. In this case, a high intensity of the background is generated by secondary electrons upon an intense excitation beam: predominance of the polynomial terms.

A similar procedure was applied for the deconvolution of the Cr 2p spectra. Here, lines for the Cr(III)-O and Cr(III)-OH were assumed together with a high-BE line for the Cr(III) satellite.

Figure 1S presents an example of the results of deconvolution without background subtraction.

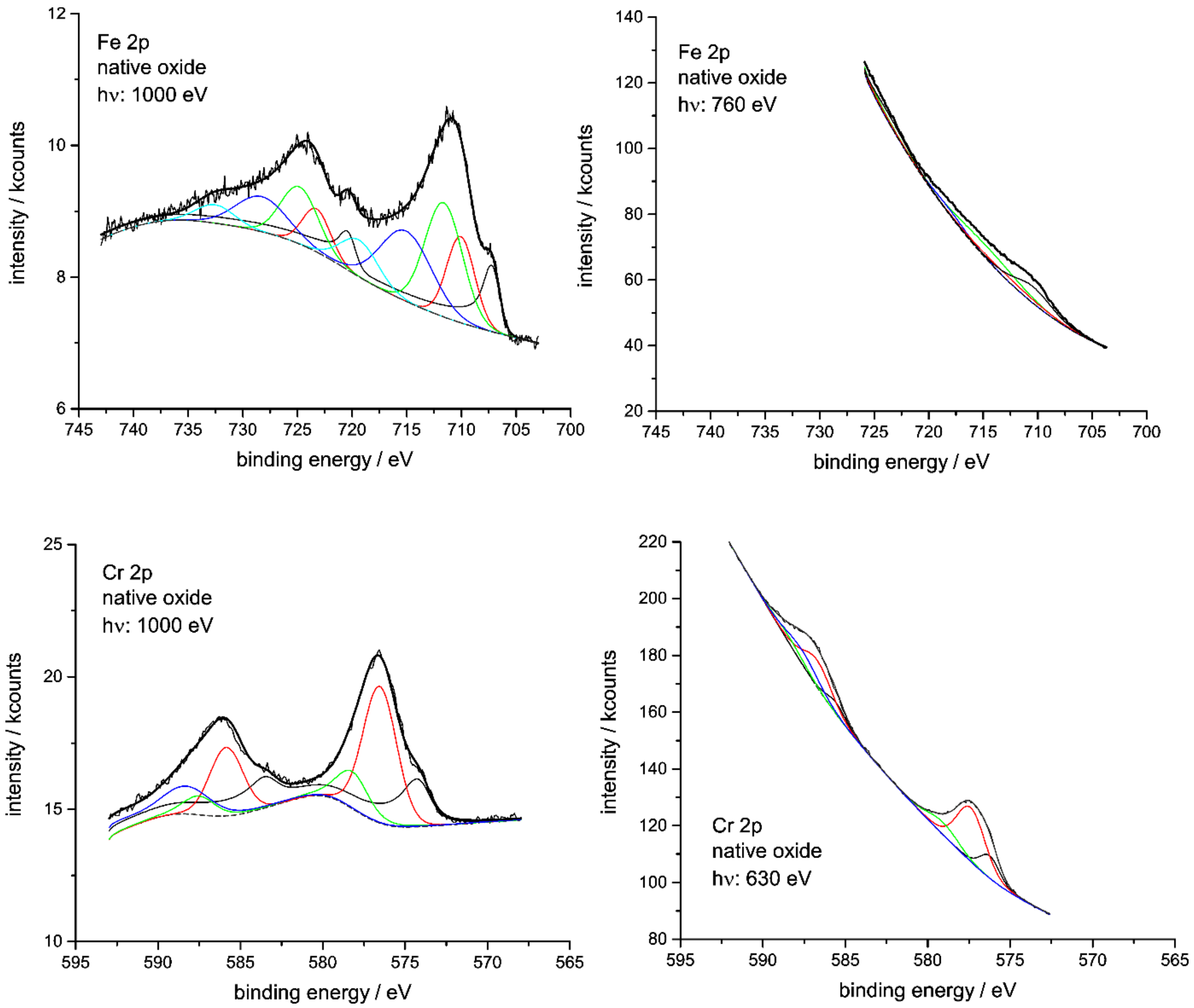

Figure S1: Fe 2p and Cr 2p core level spectra showing the results of the deconvolution with simultaneous adjustment of the background. Corrected BE.

Carbon signal: surface contamination and graphite from substrate

Figure 2S shows the surface sensitive C 1s core level spectra before and after the polarization experiment. shows a considerable attenuation of the signal, but it does not vanish. The assignment to the main signal peak at 284.9 eV can be attributed to C-C bonds. Further lines are observed at 286.3 eV and 288.6 eV, which can be attributed to C-O and O-C=O bonds respectively [1]. The presence of carbon can be ascribed to adventitious carbon but also the graphite arising from the alloy should not be excluded.

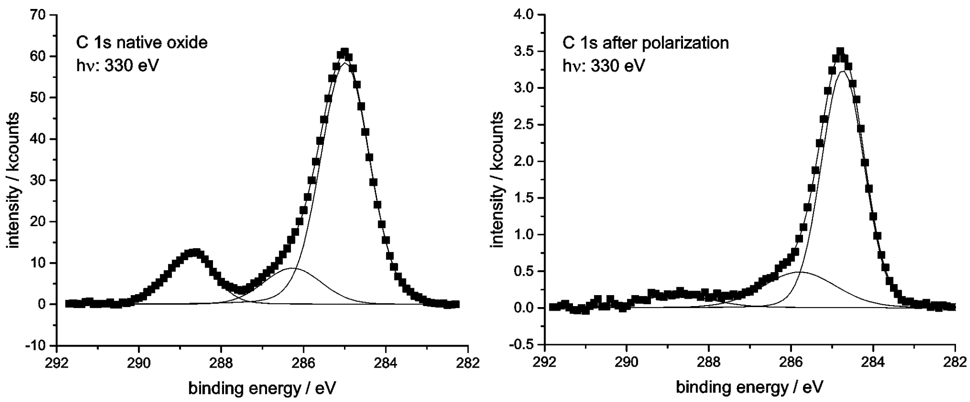

Figure S2: C1s core level spectra measured before and after the polarization experiment at an excitation energy of 330 eV.

[1] G. Greczynski, L. Hultman, Reliable determination of chemical state in x-ray photoelectron spectroscopy based on sample-work-function referencing to adventitious carbon: Resolving the myth of apparent constant binding energy of the C 1s peak, Appl. Surf. Sci. 451 (2018) 99-103.

Fe 2p 1000 eV excitation energy*

Native oxide / relative

Doublet name Fe2p_01	Peak height/ Counts	GP-FWHM/ eV	Position/ eV	LP-FWHM/ eV	Asymmetry	FWHM/ eV	abs. Area/ Counts·eV	rel. Area/ %
Doublet 1	1006.9 0.5	1.4333 1	704.0258 13.2	0.1 1	0.3 1	1.981 1.981	5008 2185	13.26 5.78
Doublet 2	1.29927 0.5	2.09679 1	3.0604 13.1999	0.1 1	0 0	3.012 3.012	4200 2100	11.12 5.56
Doublet 3	1.72034 0.5	2.78577 1	4.6307 13.1999	0.1 1	0 0	4.028 4.028	7463 3732	19.75 9.88
Doublet 4	1.06028 0.5	3.85842 1	8.0729 13.2	0.1 1	0 0	5.532 5.531	6287 3143	16.64 8.32
Doublet 5	0.55541 0.5	2.84115 1	12.3503 13.1999	0.1 1	0 0	4.089 4.089	2440 1220	6.46 3.23

After polarization / relative

Doublet name Fe2p_02	Peak height/ Counts	GP-FWHM/ eV	Position/ eV	LP-FWHM/ eV	Asymmetry	FWHM/ eV	abs. Area/ Counts·eV	rel. Area/ %
Doublet 1	1629.4 0.5	1.04698 1	703.9872 13.2	0.66492 1	0.28048 1	1.997 1.997	8359 3710	21.72 9.64
Doublet 2	0.89098 0.5	2.41107 1	2.4809 13.2	0.14302 1	0 0	2.579 2.579	4037 2021	10.49 5.25
Doublet 3	1.18583 0.5	3.14993 1	4.293 13.2	0.1 1	0 0	3.332 3.332	6895 3449	17.91 8.96
Doublet 4	0.61095 0.5	3.63567 1	7.4732 13.2	0.1 1	0 0	3.852 3.852	4110 2056	10.68 5.34
Doublet 5	0.34612 0.5	4.0462 1	11.0189 13.2	0.1 1	0 0	4.265 4.265	2571 1285	6.68 3.34

Fe 2p 760 eV excitation energy*

Native oxide / relative

Doublet name Fe2p_01	Peak height/ Counts	GP-FWHM/ eV	Position/ eV	LP-FWHM/ eV	FWHM/ eV	abs. Area/ Counts·eV	rel. Area/ %
Doublet 1	5035.6 0.5	3.2059 1	708.6371 13.2001	1.47747 1	4.069 4.069	24400 12330	22.27 11.26
Doublet 2	0.27285 0.5	2.39141 1	2.4022 13.2	0.1 1	7.784 7.748	11483 5698	10.48 5.2
Doublet 3	0.77896 0.5	2.21515 1	4.1075 13.2	0.1 1	7.186 7.184	30213 15093	27.58 13.78
Doublet 4	0.32637 0.5	1.18721 1	7.6796 13.2	0.1 1	3.885 3.885	6884 3440	6.28 3.14

After polarization / relative

Doublet name Fe2p_02	Peak height/ Counts	GP-FWHM/ eV	Position/ eV	LP-FWHM/ eV	FWHM/ eV	abs. Area/ Counts·eV	rel. Area/ %
Doublet 1	4068.7 0.5	2.25362 1	708.4227 13.2	2.72603 1	4.045 4.045	21463 10968	23.59 12.05
Doublet 2	0.42142 0.5	1.51419 1	3.2049 13.2	0.51703 1	4.228 4.228	8593 4311	9.44 4.74
Doublet 3	0.69945 0.5	3.13894 1	5.525 13.2	0.1 1	7.222 7.224	22125 11069	24.32 12.17
Doublet 4	0.32835 0.5	2.48834 1	8.2657 13.2	0.1 1	5.755 5.757	8306 4155	9.13 4.57

Cr 2p 1000 eV excitation energy*

Native oxide / relative

Doublet name Cr2p_01	Peak height/ Counts	GP-FWHM/ eV	Position/ eV	LP-FWHM/ eV	Asymmetry	FWHM/ eV	abs. Area/ Counts·eV	rel. Area/ %
Doublet 1	1801.3 0.5	1.10464 1	571.029 9.3	0.94845 1	0.32471 1	2.624 2.624	10000 4030	21.96 8.85
Doublet 2	2.86582 0.5	2.12597 1	2.5436 9.3	0.13763 0.00073	0 0	2.42 2.369	13545 6540	29.75 14.37
Doublet 3	0.77784 0.5	1.59041 1	4.2125 9.2999	0.98607 1	0 0	2.312 2.312	3961 1961	8.7 4.31
Doublet 4	0.49027 0.5	2.86601 1	14.2693 9.3	0.1 1	0 0	3.223 3.532	3062 2428	6.73 5.33

After polarization / relative

Doublet name Cr2p_01	Peak height/ Counts	GP-FWHM/ eV	Position/ eV	LP-FWHM/ eV	Asymmetry	FWHM/ eV	abs. Area/ Counts·eV	rel. Area/ %
Doublet 1	1801.3 0.5	1.10464 1	571.029 9.3	0.94845 1	0.32471 1	2.624 2.624	9999 4030	21.96 8.85
Doublet 2	2.86582 0.5	2.12597 1	2.5436 9.3	0.13763 0.00073	0 0	2.42 2.369	13544 6540	29.75 14.37
Doublet 3	0.77784 0.5	1.59041 1	4.2125 9.2999	0.98607 1	0 0	2.312 2.312	3961 1961	8.7 4.31
Doublet 4	0.49027 0.5	2.86601 1	14.2693 9.3	0.1 1	0 0	3.223 3.532	3062 2428	6.73 5.33

Cr 2p 630 eV excitation energy*

Native oxide / relative

Doublet name Cr2p_01	Peak height/ Counts	GP-FWHM/ eV	Position/ eV	LP-FWHM/ eV	FWHM/ eV	abs. Area/ Counts·eV	rel. Area/ %
Doublet 1	7872.6 0.5	1.29897 1	574.4534 9.3	0.21673 1	1.424 1.424	12628 6320	10.78 5.4
Doublet 2	2.4168 0.5	1.43271 1	1.1436 9.3	1.32234 1	2.019 2.019	43042 21539	36.75 18.39
Doublet 3	0.55949 0.5	1.67739 1	2.8321 9.3	0.1 1	2.189 2.189	10293 5146	8.79 4.39
Doublet 4	0.61822 0.5	1.7633 1	11.3782 9.3	0.1 1	2.318 2.318	12096 6044	10.33 5.16

After polarization / relative

Doublet name Cr2p_02	Peak height/ Counts	GP-FWHM/ eV	Position/ eV	LP-FWHM/ eV	FWHM/ eV	abs. Area/ Counts·eV	rel. Area/ %
Doublet 1	681.185 0.5	2.52707 1	575.6328 9.2999	0.88724 1	3.036 3.036	2430 1218	66.61 33.39

(*) values non-corrected

Calibration function

ΔBE [eV]: $2.21157 \times 10^{-4}\, h\nu$ [eV] + $2.75094 \times 10^{-6}\, h\nu^2$ [eV^2]

$BE_{corr} = BE_{meas} + \Delta BE$

Rough spectroscopic data

Native Oxide

O 1s
1000 eV

		534,45	7857,46	533,70	8172,98
		534,40	7942,14	533,65	8240,12
		534,35	8029,51	533,60	8183,06
		534,30	7941,98	533,55	8172,16
535	7823,39	534,25	8077,04	533,50	8211,17
534,95	7962,23	534,20	8033,13	533,45	8347,25
534,90	7896,40	534,15	8099,82	533,40	8123,10
534,85	7933,58	534,10	8220,70	533,35	8108,17
534,80	8038,63	534,05	8188,36	533,30	8213,37
534,75	7989,21	534	8211,07	533,25	8309,33
534,70	8057,72	533,95	8067,15	533,20	8126,32
534,65	7963,39	533,90	8077,16	533,15	8188,40
534,60	7957,77	533,85	7893,26	533,10	8315,10
534,55	7890,12	533,80	8005,14	533,05	8187,88
534,50	7913,70	533,75	8187,57	533	8160,34

532,95	8147,03	530,60	9506,22	528,25	14606,30
532,90	8270,23	530,55	9541,72	528,20	14664,40
532,85	8279,97	530,50	9646,60	528,15	14713,20
532,80	8277,07	530,45	9642,57	528,10	14911,70
532,75	8230	530,40	9796,83	528,05	15011,80
532,70	8391,98	530,35	9848,65	528	15000
532,65	8352,08	530,30	9721,17	527,95	15329,20
532,60	8267,20	530,25	9914,22	527,90	15332,30
532,55	8363,03	530,20	9954,61	527,85	15664,70
532,50	8377,37	530,15	10165,90	527,80	15778,30
532,45	8269,76	530,10	10337,30	527,75	16009,10
532,40	8212,61	530,05	10432,90	527,70	16239,90
532,35	8226,60	530	10504,80	527,65	16416,60
532,30	8234,67	529,95	10646,20	527,60	16532,60
532,25	8289,96	529,90	10796,40	527,55	16444,20
532,20	8411,26	529,85	10872,40	527,50	16610,10
532,15	8413,33	529,80	11019,60	527,45	16886,70
532,10	8313,49	529,75	11132,60	527,40	17098,20
532,05	8490,83	529,70	11464,50	527,35	17275,10
532	8524,73	529,65	11567,50	527,30	17354,30
531,95	8507,51	529,60	11727,80	527,25	17377,90
531,90	8473,43	529,55	11743,60	527,20	17331,70
531,85	8452,41	529,50	11946,40	527,15	17224,50
531,80	8627,83	529,45	12018,50	527,10	17084,60
531,75	8509,46	529,40	12069,60	527,05	17061,30
531,70	8588,02	529,35	12156,20	527	16932,40
531,65	8536,47	529,30	12522,70	526,95	16723,40
531,60	8518,18	529,25	12649,60	526,90	16629,50
531,55	8551,83	529,20	12769,90	526,85	16227,70
531,50	8728,76	529,15	12939,40	526,80	15915,50
531,45	8613,46	529,10	13057,30	526,75	15554,70
531,40	8723,33	529,05	13267,90	526,70	15142,90
531,35	8851,81	529	13162,10	526,65	14850,90
531,30	8901,60	528,95	13388,20	526,60	14328,10
531,25	8703,34	528,90	13390,80	526,55	13935,90
531,20	8684,86	528,85	13460,20	526,50	13588,90
531,15	8849,84	528,80	13851,60	526,45	12921,30
531,10	8901,03	528,75	13720,30	526,40	12486,90
531,05	9016,83	528,70	13691,90	526,35	12068,80
531	9085,31	528,65	13897,80	526,30	11917,80
530,95	9024,59	528,60	14096	526,25	11439,50
530,90	9102,58	528,55	14214,40	526,20	11089,70
530,85	9199,40	528,50	14209,20	526,15	10699,60
530,80	9135,95	528,45	14365,90	526,10	10549,60
530,75	9365,96	528,40	14382,20	526,05	10106,90
530,70	9422,93	528,35	14356,90	526	10006,70
530,65	9254,82	528,30	14387,20	525,95	9823,47

525,90	9477,63
525,85	9282,53
525,80	9020,73
525,75	9036,04
525,70	8901,40
525,65	8907,80
525,60	8638,85
525,55	8492,32
525,50	8357,50
525,45	8455,93
525,40	8329,64
525,35	8291,01
525,30	8291,36
525,25	8270,14
525,20	8282,45
525,15	8363,93
525,10	8151,20
525,05	8179,81
525	8258,63
524,95	8200,51
524,90	8112,31
524,85	8065,37
524,80	8123,15
524,75	8067,19
524,70	8113,84
524,65	8157,48
524,60	8192,77
524,55	8108,35
524,50	8175,70
524,45	8133,27
524,40	8178,58
524,35	8048,14
524,30	8035,42
524,25	8095,72
524,20	8003,47
524,15	8061,75
524,10	8029,56
524,05	8003,14
524	8125,45
523,95	8095,33
523,90	7953,70
523,85	7975,12
523,80	8137,45
523,75	8116,02
523,70	7981,70
523,65	7981,15
523,60	8022,58
523,55	8014,58
523,50	7977,54
523,45	8044,82
523,40	8054,81
523,35	8017,31
523,30	8032,55
523,25	7993,25
523,20	8099,78
523,15	8048,97
523,10	7989,84
523,05	8077,54
523	7905,92
522,95	8020,34
522,90	7973,29
522,85	8063,90
522,80	7954,04
522,75	8104,94
522,70	8063,73
522,65	8043,01
522,60	7943,79
522,55	8087,76
522,50	8128,18
522,45	8129,69
522,40	8146,78
522,35	8180,67
522,30	8096,55
522,25	7957,55
522,20	7924,11
522,15	7848,76
522,10	8064,31
522,05	7918,92
522	8020,66

Fe 2p
1000 eV

740	8485,08
739,90	8535,69
739,80	8635,74
739,70	8696,85
739,60	8555,04
739,50	8704,71
739,40	8910,73
739,30	8808,04
739,20	8739,31
739,10	8584,80
739	8838,89
738,90	8808,60
738,80	8876,33
738,70	8786,17
738,60	8714,44
738,50	8713,46
738,40	8809,45
738,30	8740,42
738,20	8925,66
738,10	8838,62
738	8791,08
737,90	8809,01
737,80	8791,54
737,70	8716,10
737,60	8775,08
737,50	8817,04
737,40	8866,41
737,30	8811,25
737,20	8743,56
737,10	8698,17
737	8708,48
736,90	8840,92
736,80	8902,92
736,70	8734,92
736,60	8841,16
736,50	8882,96
736,40	8907,45
736,30	8835,84
736,20	8928,22
736,10	8977,95
736	8861,20
735,90	8888,73
735,80	8955,33
735,70	8851,35
735,60	8950,99

735,50	8891,23	730,80	9153,29	726,10	9535,45
735,40	8944,42	730,70	9090,93	726	9372,75
735,30	8939,79	730,60	9184,78	725,90	9327,29
735,20	8839,75	730,50	9223,72	725,80	9470,71
735,10	8962,39	730,40	9318,47	725,70	9528,95
735	8827,31	730,30	9299,34	725,60	9464,06
734,90	8864,63	730,20	9098,45	725,50	9617,83
734,80	8848,49	730,10	9283,35	725,40	9457,83
734,70	9036,51	730	9270,50	725,30	9424,09
734,60	8930,98	729,90	9325,25	725,20	9515,98
734,50	8804,48	729,80	9254,76	725,10	9663,84
734,40	8982,68	729,70	9254,22	725	9488,86
734,30	8885,23	729,60	9134,93	724,90	9536,40
734,20	9051,20	729,50	9136,84	724,80	9489,92
734,10	8884,73	729,40	9339,07	724,70	9488,13
734	8947,86	729,30	9257,43	724,60	9609,56
733,90	8994,19	729,20	9177,80	724,50	9590,31
733,80	9059,93	729,10	9259,34	724,40	9658,08
733,70	8993,24	729	9307,34	724,30	9645,87
733,60	9105,96	728,90	9270,54	724,20	9593,73
733,50	9060,95	728,80	9273,06	724,10	9629,43
733,40	9020,68	728,70	9535,67	724	9750,85
733,30	9061,60	728,60	9247,08	723,90	9769,32
733,20	9024,16	728,50	9244,63	723,80	9665,46
733,10	8967,76	728,40	9230,46	723,70	9592,71
733	9032,80	728,30	9242,03	723,60	9680,76
732,90	8967,66	728,20	9303,30	723,50	9753,78
732,80	9065,29	728,10	9363,61	723,40	9812,34
732,70	9143,50	728	9277,66	723,30	9874,92
732,60	9034,99	727,90	9264,97	723,20	9790,28
732,50	9054,63	727,80	9374,46	723,10	9708,72
732,40	9095,01	727,70	9369,48	723	9844,86
732,30	9061,64	727,60	9250,92	722,90	9916,49
732,20	9001,56	727,50	9393,65	722,80	9856,78
732,10	9180,23	727,40	9327,63	722,70	9953,67
732	9151,19	727,30	9355,19	722,60	9977,51
731,90	9096,45	727,20	9465,93	722,50	10016,60
731,80	9183,60	727,10	9402,69	722,40	9907,17
731,70	9203,12	727	9375,69	722,30	9991,79
731,60	9216,86	726,90	9406,45	722,20	10016,80
731,50	9183,53	726,80	9439,49	722,10	10164,30
731,40	9309,37	726,70	9443,65	722	10119,70
731,30	9117,08	726,60	9447,97	721,90	9966,98
731,20	9133,11	726,50	9219,93	721,80	10014,80
731,10	9227,40	726,40	9472,38	721,70	9972,26
731	9093,77	726,30	9344,50	721,60	10050,20
730,90	8896,48	726,20	9405,17	721,50	9956,61

721,40	10019,30	716,70	9186,57	712	9029,27
721,30	9958,74	716,60	9017,13	711,90	9042,37
721,20	9866,13	716,50	9214,99	711,80	9109,83
721,10	10199,70	716,40	9052,72	711,70	9128,14
721	10136,50	716,30	9008,75	711,60	9277,32
720,90	9961,01	716,20	9054,09	711,50	9203,01
720,80	10013,90	716,10	9003,43	711,40	9172,91
720,70	9936,61	716	9084,59	711,30	9162,64
720,60	9892,55	715,90	8926,40	711,20	9245,40
720,50	9747,70	715,80	9033,44	711,10	9335,49
720,40	9718,23	715,70	8990,17	711	9438,75
720,30	9826,88	715,60	8906,39	710,90	9359,53
720,20	9813,30	715,50	8774,53	710,80	9436,74
720,10	9753,68	715,40	8824,59	710,70	9353,28
720	9716,52	715,30	9049,60	710,60	9358,02
719,90	9733,36	715,20	8952,98	710,50	9462,22
719,80	9674,73	715,10	8753,67	710,40	9530,30
719,70	9744,47	715	8870,67	710,30	9592,26
719,60	9672,53	714,90	8869,11	710,20	9629,52
719,50	9559,99	714,80	8886,14	710,10	9649,90
719,40	9497,03	714,70	8758,05	710	9864,97
719,30	9578,49	714,60	8804,81	709,90	9809,63
719,20	9561,95	714,50	8833,65	709,80	9777,72
719,10	9338,90	714,40	8961,92	709,70	9728,39
719	9358,09	714,30	8967,22	709,60	9848,50
718,90	9355,25	714,20	8889,32	709,50	9931,57
718,80	9394,66	714,10	8955,27	709,40	10096,10
718,70	9306,15	714	8949,96	709,30	10053,10
718,60	9219,67	713,90	8781,91	709,20	9977,16
718,50	9252,37	713,80	8898,45	709,10	10167,80
718,40	9260,39	713,70	9026,03	709	10290,40
718,30	9235,90	713,60	8972,24	708,90	10104
718,20	9391,12	713,50	8967,49	708,80	10063,20
718,10	9084,84	713,40	8872,30	708,70	10239,20
718	9304,25	713,30	8875,35	708,60	10310,80
717,90	9174,84	713,20	9024,55	708,50	10360,20
717,80	9183,25	713,10	8943,42	708,40	10593,90
717,70	9190,07	713	8924,70	708,30	10529,50
717,60	9293,01	712,90	8891,80	708,20	10293,40
717,50	9321,09	712,80	8894,41	708,10	10472,90
717,40	9352,13	712,70	9155,97	708	10375,80
717,30	9184,96	712,60	9095,32	707,90	10353,70
717,20	9360,91	712,50	9124,43	707,80	10525,90
717,10	9247,17	712,40	8920,17	707,70	10321,50
717	9231,07	712,30	8997,12	707,60	10376
716,90	9265,29	712,20	9022,87	707,50	10361,90
716,80	9252,56	712,10	9077,78	707,40	10305,50

707,30	10334,20
707,20	10298,30
707,10	10183,30
707	9994,93
706,90	9907,08
706,80	9912,14
706,70	9820,82
706,60	9766,61
706,50	9706,45
706,40	9470,10
706,30	9323,57
706,20	9219,22
706,10	9081,59
706	9027,45
705,90	8880,16
705,80	8907,18
705,70	8769,89
705,60	8802,38
705,50	8592,87
705,40	8637,74
705,30	8491,61
705,20	8547,97
705,10	8520,31
705	8431,39
704,90	8417,91
704,80	8461,07
704,70	8410,05
704,60	8345,22
704,50	8363,40
704,40	8509,97

704,30	8305,70
704,20	8294,38
704,10	8274,39
	8236,80
704	
703,90	8242,49
703,80	8077,61
703,70	7935,15
703,60	7738,48
703,50	7646,61
703,40	7671,64
703,30	7483,46
703,20	7396,64
703,10	7303,95
703	7231,66
702,90	7339,12
702,80	7217,33
702,70	7152,70
702,60	7055,86
702,50	7134,87
702,40	7027,44
702,30	7033,10
702,20	7039,94
702,10	6992,53
702	7124,41
701,90	6970,39
701,80	6982,66
701,70	7114,54
701,60	7004,87
701,50	7118,37

701,40	7039,06
701,30	7058,18
701,20	7081
701,10	7111,37
701	7052,54
700,90	7106,11
700,80	7067,17
700,70	7083,40
700,60	7030,81
700,50	7026,48
700,40	7002,47
700,30	6903,21
700,20	6967,66
700,10	7069,18
700	7100,79

Cr 2p
1000 eV

590	14638,70
589,90	14824
589,80	14711,90
589,70	14836,90
589,60	14753,90
589,50	14758
589,40	14761,80
589,30	15042,40
589,20	15026,90
589,10	15041,50
589	15037,30
588,90	14913,60
588,80	15124,60
588,70	15163
588,60	14968,60
588,50	15115,20

588,40	15251,10
588,30	15527,10
588,20	15575,20
588,10	15365,30
588	15504,40
587,90	15432,10
587,80	15513,50
587,70	15416,20
587,60	15655,30
587,50	15630,60
587,40	15567,60
587,30	15648,60
587,20	15653,10
587,10	15946,20
587	15920,80
586,90	15791,40
586,80	16071,80

586,70	16119,90
586,60	16006,50
586,50	15951,70
586,40	15972
586,30	16262,10
586,20	16206,60
586,10	16427,90
586	16435,40
585,90	16396,50
585,80	16531,20
585,70	16558,10
585,60	16863,40
585,50	16720,60
585,40	16794,20
585,30	16873,30
585,20	17093
585,10	17244,60

585	17266,10	580,30	16443,40	575,60	17713,30
584,90	17200,50	580,20	16372,20	575,50	17878,30
584,80	17393,50	580,10	16263,70	575,40	18002,30
584,70	17309,50	580	16450,50	575,30	18003,40
584,60	17484,10	579,90	16239,30	575,20	18438,70
584,50	17698	579,80	16236,60	575,10	18699,30
584,40	17678,20	579,70	16320,80	575	18792,30
584,30	17949,80	579,60	16178,30	574,90	18974,20
584,20	17920,40	579,50	16128,70	574,80	19301,60
584,10	18055,60	579,40	16223,60	574,70	19523,90
584	18107,60	579,30	16208,20	574,60	19674,80
583,90	18163,80	579,20	16036,20	574,50	19927,50
583,80	18259,30	579,10	16129,20	574,40	19997,60
583,70	18327,50	579	15846,80	574,30	20275,70
583,60	18204,20	578,90	16003,40	574,20	20344,40
583,50	18357,40	578,80	15981,20	574,10	20319,30
583,40	18463,70	578,70	16046,60	574	20352,20
583,30	18501,80	578,60	15921,90	573,90	20623,40
583,20	18292,70	578,50	16077	573,80	20784,30
583,10	18468,30	578,40	16086,60	573,70	20925,60
583	18370,40	578,30	15955,90	573,60	21020,60
582,90	18391,30	578,20	16183,10	573,50	20822,80
582,80	18210,80	578,10	16128,90	573,40	20617,40
582,70	18092,90	578	16005,40	573,30	20556,50
582,60	18076,90	577,90	15947,70	573,20	20394,30
582,50	17949,70	577,80	16076,70	573,10	20195,30
582,40	17713	577,70	16007,70	573	20076,40
582,30	17577,50	577,60	16145,40	572,90	19783,80
582,20	17497,10	577,50	16094	572,80	19672,10
582,10	17410,40	577,40	16247	572,70	19451,50
582	17211,40	577,30	16294,30	572,60	19139,60
581,90	17196,80	577,20	16203,90	572,50	18648,50
581,80	17088	577,10	16234,40	572,40	18569,80
581,70	17082,80	577	16425,90	572,30	18356,90
581,60	17043,20	576,90	16377,10	572,20	18226
581,50	16998,40	576,80	16526,80	572,10	17645,70
581,40	16902,40	576,70	16616,50	572	17256,40
581,30	16813,90	576,60	16740,90	571,90	17417,60
581,20	16688,20	576,50	16765	571,80	17155,10
581,10	16670,60	576,40	16701,70	571,70	16787,30
581	16665,40	576,30	16922,90	571,60	16670
580,90	16727,70	576,20	17009,50	571,50	16678,80
580,80	16632,20	576,10	17143,30	571,40	16602,40
580,70	16513,50	576	17129,70	571,30	16581,20
580,60	16391,90	575,90	17309,60	571,20	16410
580,50	16502,20	575,80	17537,40	571,10	16400
580,40	16754,70	575,70	17570,90	571	16483,50

570,90	16355,40	568,90	14567	566,90	14482,70
570,80	16133,40	568,80	14585,80	566,80	14757,30
570,70	15747,60	568,70	14505,90	566,70	14549,10
570,60	15645,60	568,60	14613,60	566,60	14751,10
570,50	15720	568,50	14625,90	566,50	14773,20
570,40	15586,70	568,40	14478,60	566,40	14702,60
570,30	15385,10	568,30	14579	566,30	14519,70
570,20	15196,80	568,20	14629,20	566,20	14705,90
570,10	14903,80	568,10	14548,10	566,10	14697,70
570	14870,60	568	14430,40	566	14695,80
569,90	14815,40	567,90	14475,50	565,90	14644,90
569,80	14734,60	567,80	14515,90	565,80	14684,70
569,70	14780,60	567,70	14636,30	565,70	14597,30
569,60	14736	567,60	14713,30	565,60	14793,90
569,50	14609,90	567,50	14599,50	565,50	14745,30
569,40	14753,60	567,40	14553,10	565,40	14841,10
569,30	14687,60	567,30	14571,60	565,30	14682,40
569,20	14582	567,20	14493,70	565,20	14574,40
569,10	14499,50	567,10	14606,10	565,10	14564,60
569	14504,10	567	14670,10	565	14696,20

Cr 3s
100 eV

		75,70	7337720,00	74,10	7466320,00
		75,60	7323070,00	74	7400550,00
		75,50	7312890,00	73,90	7307270,00
77	7714930,00	75,40	7311810,00	73,80	7207800,00
76,90	7685930,00	75,30	7321590,00	73,70	7094520,00
76,80	7652730,00	75,20	7336760,00	73,60	6964070,00
76,70	7618580,00	75,10	7355510,00	73,50	6840420,00
76,60	7581590,00	75	7384080,00	73,40	6717770,00
76,50	7546240,00	74,90	7417320,00	73,30	6597050,00
76,40	7514290,00	74,80	7447390,00	73,20	6492780,00
76,30	7482730,00	74,70	7481610,00	73,10	6400030,00
76,20	7454090,00	74,60	7515740,00	73	6316740,00
76,10	7424710,00	74,50	7539200,00	72,90	6242480,00
76	7399820,00	74,40	7549700,00	72,80	6183410,00
75,90	7374940,00	74,30	7541620,00	72,70	6130090,00
75,80	7354170,00	74,20	7516710,00	72,60	6083100,00

72,50	6042050,00	72,30	5968010,00	72,10	5901400,00
72,40	6006320,00	72,20	5934040,00	72	5871010,00

Fe 2p
760 eV

		736,40	312552	732,30	217487
		736,30	309333	732,20	216267
		736,20	306691	732,10	214052
		736,10	304372	732	212651
		736	301294	731,90	210551
740	468933	735,90	298038	731,80	208192
739,90	463723	735,80	295036	731,70	207089
739,80	458084	735,70	292953	731,60	205493
739,70	451955	735,60	289036	731,50	204946
739,60	445799	735,50	286729	731,40	203223
739,50	439369	735,40	284447	731,30	201126
739,40	434935	735,30	281294	731,20	199575
739,30	429772	735,20	277909	731,10	198227
739,20	423973	735,10	276323	731	196750
739,10	419806	735	273710	730,90	195703
739	414596	734,90	271619	730,80	194488
738,90	410167	734,80	268882	730,70	192755
738,80	404841	734,70	266614	730,60	190775
738,70	400706	734,60	264669	730,50	189685
738,60	394870	734,50	263072	730,40	188603
738,50	390721	734,40	260423	730,30	186967
738,40	386622	734,30	257567	730,20	185845
738,30	382234	734,20	255281	730,10	184359
738,20	378148	734,10	253122	730	183006
738,10	372616	734	251069	729,90	181238
738	368917	733,90	248721	729,80	179985
737,90	365257	733,80	246578	729,70	178946
737,80	361681	733,70	243985	729,60	177911
737,70	357521	733,60	242404	729,50	176739
737,60	353661	733,50	240310	729,40	175825
737,50	350303	733,40	238318	729,30	174291
737,40	346135	733,30	236061	729,20	172733
737,30	342685	733,20	233906	729,10	171557
737,20	338848	733,10	232644	729	170589
737,10	335565	733	230871	728,90	169559
737	332768	732,90	228841	728,80	168497
736,90	329878	732,80	226881	728,70	167278
736,80	325370	732,70	224903	728,60	166119
736,70	322486	732,60	223951	728,50	164913
736,60	319693	732,50	221223	728,40	163977
736,50	315624	732,40	219981	728,30	162602

728,20	161423	723,50	122235	718,80	93504,60
728,10	160806	723,40	122091	718,70	93270,80
728	159894	723,30	121374	718,60	92506,80
727,90	158433	723,20	119709	718,50	91639
727,80	157270	723,10	119410	718,40	92235,30
727,70	156589	723	119059	718,30	91836,50
727,60	155399	722,90	118655	718,20	91315,90
727,50	154290	722,80	117555	718,10	91024,90
727,40	154200	722,70	117031	718	90045,70
727,30	152159	722,60	116105	717,90	89908,10
727,20	151251	722,50	115927	717,80	89076,80
727,10	150403	722,40	114960	717,70	89022,20
727	149795	722,30	114740	717,60	88603,40
726,90	148421	722,20	113476	717,50	88148,20
726,80	147561	722,10	112808	717,40	88078,50
726,70	147272	722	112464	717,30	87929,20
726,60	146064	721,90	111619	717,20	87542,70
726,50	144712	721,80	111268	717,10	86901,70
726,40	144142	721,70	109964	717	86745,20
726,30	143440	721,60	109840	716,90	86335,40
726,20	142321	721,50	109820	716,80	85899,90
726,10	141565	721,40	109122	716,70	85576,20
726	141265	721,30	108042	716,60	85230,60
725,90	140518	721,20	107393	716,50	85063,20
725,80	139566	721,10	106528	716,40	84210,10
725,70	138613	721	105728	716,30	83841,50
725,60	137679	720,90	105094	716,20	83628,30
725,50	136426	720,80	104887	716,10	83695
725,40	135674	720,70	104165	716	83229,30
725,30	135209	720,60	103684	715,90	82749,50
725,20	134160	720,50	102695	715,80	82314,90
725,10	133300	720,40	101891	715,70	81431,70
725	132468	720,30	101649	715,60	81279
724,90	132091	720,20	100883	715,50	80883,90
724,80	131461	720,10	100346	715,40	80836,40
724,70	130447	720	99308,90	715,30	80487
724,60	129867	719,90	99036,20	715,20	79728,70
724,50	129016	719,80	98327,10	715,10	79494,30
724,40	128359	719,70	98270,80	715	79300,10
724,30	128042	719,60	97736,80	714,90	78992,30
724,20	126546	719,50	96967,70	714,80	78433,50
724,10	126267	719,40	95781,60	714,70	78086,90
724	125582	719,30	95447,60	714,60	78073,20
723,90	124844	719,20	95580,40	714,50	77753,50
723,80	124102	719,10	95429	714,40	77415,70
723,70	123728	719	94007,60	714,30	76755,50
723,60	122205	718,90	93971	714,20	76664,60

714,10	76442,80	709,40	62931	704,70	44908,40
714	75894,30	709,30	62569,30	704,60	44598,50
713,90	75781,80	709,20	62170,10	704,50	44475,80
713,80	75103,30	709,10	62002,20	704,40	44420,40
713,70	74835,90	709	61702,50	704,30	44074
713,60	74631,90	708,90	61401,60	704,20	43642,10
713,50	74318,80	708,80	61423,10	704,10	43367,10
713,40	73687	708,70	60399,20	704	43279,20
713,30	73370,70	708,60	59920,90	703,90	42612,80
713,20	73257,80	708,50	59944,20	703,80	42957,60
713,10	72624,10	708,40	59687,50	703,70	42755,80
713	72340,70	708,30	59486	703,60	42373,40
712,90	72169,10	708,20	58994,90	703,50	42271
712,80	71977,90	708,10	58897,70	703,40	41945
712,70	71282,70	708	58470,40	703,30	41810,50
712,60	71198,10	707,90	57720	703,20	41769,10
712,50	70439,90	707,80	57354,80	703,10	41193,80
712,40	70817,10	707,70	56982,20	703	41151,40
712,30	70502,80	707,60	56538	702,90	40927,60
712,20	70400,10	707,50	55780,30	702,80	40807,10
712,10	69645	707,40	55120,80	702,70	40510,70
712	69338,40	707,30	54380,90	702,60	40382,50
711,90	68874,50	707,20	53721,20	702,50	40285,40
711,80	68595,90	707,10	53696,50	702,40	40096,40
711,70	68489,10	707	53450,90	702,30	40051,30
711,60	67733	706,90	53016,60	702,20	39682,80
711,50	67855,40	706,80	52443	702,10	39381,30
711,40	67531,30	706,70	51578,30	702	39521,30
711,30	67808,60	706,60	51564,20	701,90	39469,60
711,20	67248,40	706,50	50872,50	701,80	38992,40
711,10	66871,60	706,40	50705,80	701,70	39008
711	66224,80	706,30	50057	701,60	38988,50
710,90	66259	706,20	49850,50	701,50	38345,90
710,80	65981,20	706,10	49381,90	701,40	38159,20
710,70	65811,90	706	48931	701,30	38330,60
710,60	65075,90	705,90	48391,60	701,20	38368,80
710,50	64992,20	705,80	48273,30	701,10	38239,80
710,40	65364,10	705,70	48299	701	37953,60
710,30	64949,50	705,60	47889,70	700,90	37778,90
710,20	64755,10	705,50	47077,60	700,80	37608,80
710,10	64528	705,40	46742,50	700,70	37180,10
710	64410,20	705,30	46631,80	700,60	37118,10
709,90	63943,70	705,20	46500	700,50	37069,80
709,80	63728,90	705,10	46107,60	700,40	37093,90
709,70	63462,40	705	45863,80	700,30	36961,50
709,60	63465,30	704,90	45587,30	700,20	36869,80
709,50	63056,90	704,80	45287,60	700,10	36769,50

700	36655,90

O 1s
580 eV

540	125995
539,90	125515
539,80	124995
539,70	123703
539,60	122931
539,50	122756
539,40	121828
539,30	121025
539,20	121081
539,10	120098
539	119583
538,90	118990
538,80	118755
538,70	117609
538,60	116815
538,50	116996
538,40	115827
538,30	115251
538,20	115167
538,10	114017
538	113521
537,90	113274
537,80	112232
537,70	111525
537,60	111338
537,50	110627
537,40	109932
537,30	109396
537,20	108862
537,10	108162
537	108291
536,90	107876
536,80	106547
536,70	105538
536,60	105588
536,50	104524
536,40	104504
536,30	104004
536,20	103353
536,10	102393
536	101875
535,90	101696
535,80	101290
535,70	100520
535,60	99811,90
535,50	99816,30
535,40	98946,30
535,30	98433
535,20	97731,10
535,10	97202,10
535	96635,80
534,90	96235,40
534,80	95885,90
534,70	95222,30
534,60	95857
534,50	95051,70
534,40	94004,10
534,30	93388,10
534,20	93880,80
534,10	93119
534	92552,80
533,90	92347,30
533,80	92392
533,70	92629,10
533,60	92030,30
533,50	91987,60
533,40	91940
533,30	91858
533,20	91906,60
533,10	92192
533	92669,40
532,90	92707,50
532,80	93378
532,70	93698,40
532,60	94320,10
532,50	94859,10
532,40	96332,60
532,30	97437,10
532,20	98659
532,10	100504
532	102243
531,90	105195
531,80	107678
531,70	110744
531,60	114214
531,50	118141
531,40	122289
531,30	126047
531,20	130274
531,10	134145
531	136906
530,90	139910
530,80	141415
530,70	142004
530,60	142473
530,50	141647
530,40	140198
530,30	138123
530,20	135777
530,10	133369
530	131061
529,90	129135
529,80	126838
529,70	126424
529,60	127338
529,50	128569
529,40	131161
529,30	133651
529,20	136828
529,10	137908
529	139156
528,90	137838
528,80	135758
528,70	130904
528,60	124565

528,50	116992	527,30	63291,10	526,10	58615,90
528,40	109128	527,20	62669,20	526	58427,30
528,30	100946	527,10	62168	525,90	57956,80
528,20	92938,90	527	61766,50	525,80	57221
528,10	86005,60	526,90	61012,30	525,70	57050,80
528	80100,90	526,80	60821,50	525,60	56901,60
527,90	75230,20	526,70	60446,30	525,50	56632,40
527,80	71867	526,60	59820,10	525,40	56169,90
527,70	69136,90	526,50	59682,10	525,30	55863,20
527,60	66784	526,40	59577,50	525,20	55518,80
527,50	65140	526,30	58956,20	525,10	55564,50
527,40	64443,20	526,20	58647,10	525	55221,40

Cr 2p
630 eV

		597,50	335113	594,70	284003
		597,40	334569	594,60	282341
		597,30	331442	594,50	280780
600	384131	597,20	329744	594,40	279415
599,90	382573	597,10	327430	594,30	277387
599,80	380523	597	326638	594,20	275561
599,70	379533	596,90	323917	594,10	274597
599,60	377389	596,80	322159	594	271793
599,50	375021	596,70	320280	593,90	269896
599,40	372914	596,60	318759	593,80	269367
599,30	371467	596,50	316530	593,70	266959
599,20	369260	596,40	314664	593,60	265078
599,10	367083	596,30	312455	593,50	263709
599	365557	596,20	310935	593,40	262504
598,90	363454	596,10	309636	593,30	261367
598,80	360841	596	306998	593,20	259161
598,70	358421	595,90	305706	593,10	257482
598,60	356870	595,80	304446	593	256008
598,50	354675	595,70	301599	592,90	253847
598,40	352534	595,60	300575	592,80	252934
598,30	352168	595,50	299018	592,70	251629
598,20	348794	595,40	296360	592,60	249690
598,10	346157	595,30	295121	592,50	248173
598	344381	595,20	292774	592,40	245956
597,90	342801	595,10	291452	592,30	244585
597,80	341190	595	289825	592,20	242735
597,70	339132	594,90	287864	592,10	242545
597,60	336866	594,80	285975	592	241974

591,90	239997	587,20	194289	582,50	151288
591,80	238492	587,10	193790	582,40	150439
591,70	236994	587	192468	582,30	149268
591,60	236064	586,90	191727	582,20	148557
591,50	234506	586,80	191953	582,10	147638
591,40	233095	586,70	191687	582	147451
591,30	231480	586,60	190788	581,90	146791
591,20	231101	586,50	190745	581,80	146383
591,10	229302	586,40	190801	581,70	144713
591	228051	586,30	189440	581,60	143944
590,90	227113	586,20	190073	581,50	143274
590,80	225700	586,10	189358	581,40	142823
590,70	225600	586	188764	581,30	142140
590,60	222977	585,90	188421	581,20	141830
590,50	222465	585,80	188250	581,10	140945
590,40	221814	585,70	188031	581	139704
590,30	220402	585,60	187911	580,90	139551
590,20	218852	585,50	187021	580,80	138595
590,10	217988	585,40	186513	580,70	138074
590	217399	585,30	186448	580,60	137209
589,90	216387	585,20	185237	580,50	136585
589,80	215043	585,10	185172	580,40	135680
589,70	213731	585	183918	580,30	135655
589,60	213079	584,90	182889	580,20	135056
589,50	212340	584,80	182744	580,10	134119
589,40	211057	584,70	180414	580	133572
589,30	210105	584,60	178792	579,90	132977
589,20	209332	584,50	178014	579,80	131869
589,10	208187	584,40	177159	579,70	130976
589	207336	584,30	175171	579,60	130935
588,90	206981	584,20	173177	579,50	130327
588,80	205433	584,10	171832	579,40	129836
588,70	204589	584	169982	579,30	129428
588,60	203519	583,90	168308	579,20	128901
588,50	202895	583,80	167570	579,10	128705
588,40	202638	583,70	166142	579	128252
588,30	201391	583,60	164958	578,90	127343
588,20	200613	583,50	162915	578,80	127273
588,10	199714	583,40	161137	578,70	126762
588	199432	583,30	160058	578,60	125999
587,90	198547	583,20	158777	578,50	126308
587,80	197399	583,10	157075	578,40	125883
587,70	197118	583	156824	578,30	125320
587,60	196654	582,90	155416	578,20	125685
587,50	195872	582,80	154602	578,10	125586
587,40	195702	582,70	153174	578	124833
587,30	195495	582,60	152338	577,90	124886

577,80	124848	573,50	100756	569,20	84080,60
577,70	124436	573,40	99654,60	569,10	84074,40
577,60	124339	573,30	99352,70	569	83418,10
577,50	124495	573,20	97885	568,90	83340
577,40	124180	573,10	97449,80	568,80	83316,60
577,30	123999	573	97296,20	568,70	83484,30
577,20	124194	572,90	96558,40	568,60	82801
577,10	124238	572,80	95383,90	568,50	82370,50
577	125146	572,70	95146,30	568,40	82154,50
576,90	124713	572,60	94831,80	568,30	81981,50
576,80	125016	572,50	94399,50	568,20	81991,60
576,70	125361	572,40	94162,70	568,10	81612,20
576,60	125782	572,30	93824	568	81404,40
576,50	126738	572,20	93112,80	567,90	81345,60
576,40	126843	572,10	92632	567,80	80747,90
576,30	127584	572	92653	567,70	80381,70
576,20	128127	571,90	92439,40	567,60	80351,90
576,10	128262	571,80	91444,10	567,50	80124,40
576	128444	571,70	91094,70	567,40	80482,50
575,90	128151	571,60	90996,70	567,30	79847,80
575,80	128964	571,50	90837,30	567,20	79589,90
575,70	129090	571,40	90505,80	567,10	79256
575,60	128074	571,30	90329	567	79153,60
575,50	127974	571,20	89974,10	566,90	78666,50
575,40	127809	571,10	89847,30	566,80	78940,80
575,30	126497	571	88908,20	566,70	78408,30
575,20	126232	570,90	88895,50	566,60	78417,10
575,10	125173	570,80	88687	566,50	78247
575	123922	570,70	88416,60	566,40	77866,50
574,90	123509	570,60	87981,70	566,30	77696,90
574,80	122490	570,50	87383,60	566,20	77532,90
574,70	121210	570,40	87051,70	566,10	77537,30
574,60	119946	570,30	86784,50	566	77582,60
574,50	118720	570,20	87169,20	565,90	77494,20
574,40	117451	570,10	86430,50	565,80	77127,70
574,30	115266	570	86450,40	565,70	76571,20
574,20	113166	569,90	86452,90	565,60	76045,30
574,10	110782	569,80	86074,40	565,50	76105,50
574	109185	569,70	85499,90	565,40	76075,20
573,90	107391	569,60	85303,60	565,30	75786,90
573,80	105020	569,50	84956,40	565,20	75427,70
573,70	103642	569,40	85508,90	565,10	75794
573,60	102113	569,30	84726,90	565	76067,60

After Polarization

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O 1s

1000 eV

535	7552,71
534,95	7621,58
534,90	7456,41
534,85	7525,75
534,80	7608,44
534,75	7545,87
534,70	7551,12
534,65	7687,60
534,60	7616,15
534,55	7627,93
534,50	7536,09
534,45	7610,55
534,40	7652,63
534,35	7597,97
534,30	7574,30
534,25	7679,67
534,20	7600,35
534,15	7618,51
534,10	7644,58
534,05	7646,69
534	7667,60
533,95	7718,71
533,90	7814,30
533,85	7681,12
533,80	7624,11
533,75	7697,90
533,70	7718,54
533,65	7708,80
533,60	7738
533,55	7555,41
533,50	7555,57
533,45	7711,19
533,40	7739,49
533,35	7702,43
533,30	7824,02
533,25	7864,28
533,20	7670,45
533,15	7702,26
533,10	7757,66
533,05	7761,34
533	7767,35
532,95	7801,32
532,90	7747,67
532,85	7837,39

532,80	7804,56	530,45	9372,19	528,10	13671,40
532,75	7767,19	530,40	9426,56	528,05	13634,30
532,70	7736,59	530,35	9649,77	528	13590,40
532,65	7703,25	530,30	9680,09	527,95	13527
532,60	7786,98	530,25	9815,58	527,90	13618,60
532,55	7741,62	530,20	9968	527,85	13488,10
532,50	7738,51	530,15	9882,55	527,80	13421,60
532,45	7871,42	530,10	10172,10	527,75	13493
532,40	8003,19	530,05	10301,30	527,70	13498,30
532,35	7750,82	530	10373,10	527,65	13575
532,30	7751,46	529,95	10345,60	527,60	13399,80
532,25	7787	529,90	10611,10	527,55	13390,70
532,20	7835,21	529,85	10896,40	527,50	13456,90
532,15	7784,99	529,80	11001,20	527,45	13185,40
532,10	7941,81	529,75	11123,20	527,40	13221,80
532,05	7804,85	529,70	11243,30	527,35	13288,60
532	7832,94	529,65	11265,90	527,30	13100,70
531,95	7931,43	529,60	11366,80	527,25	13106,30
531,90	7871,74	529,55	11609,30	527,20	13094,50
531,85	7884	529,50	11630,50	527,15	12805,90
531,80	8077,55	529,45	11939,20	527,10	12671,50
531,75	8131,56	529,40	12204,30	527,05	12560
531,70	8043,76	529,35	12341,90	527	12574,80
531,65	8050,24	529,30	12380,50	526,95	12276,80
531,60	8174,53	529,25	12521,30	526,90	12265,30
531,55	8133,13	529,20	12548,10	526,85	12188,30
531,50	8130,69	529,15	12649,20	526,80	12104,90
531,45	8311,54	529,10	12961,70	526,75	11655,80
531,40	8422,01	529,05	12937,10	526,70	11499,10
531,35	8410,39	529	12977,30	526,65	11353,90
531,30	8457,56	528,95	13230,20	526,60	11027,30
531,25	8448,34	528,90	13345,80	526,55	10905,80
531,20	8573,86	528,85	13406,30	526,50	10716,30
531,15	8484,31	528,80	13539,70	526,45	10490,40
531,10	8524,14	528,75	13558,60	526,40	10336
531,05	8602,34	528,70	13580,50	526,35	10075,70
531	8579,02	528,65	13805,50	526,30	9908,63
530,95	8755,61	528,60	13821,10	526,25	9623,12
530,90	8909,12	528,55	13773,60	526,20	9501,60
530,85	8862,58	528,50	13778	526,15	9385,56
530,80	8907,06	528,45	13733,30	526,10	9324,22
530,75	9019,48	528,40	13608,90	526,05	9033,91
530,70	9054,68	528,35	13648,40	526	8808,60
530,65	8973,52	528,30	13621,20	525,95	8727,02
530,60	9162,11	528,25	13568	525,90	8771,52
530,55	9348,65	528,20	13657,50	525,85	8682,68
530,50	9362,87	528,15	13708,40	525,80	8462,97

525,75	8376,78	524,45	7584,74	523,15	7503,21
525,70	8377,87	524,40	7562,39	523,10	7660,92
525,65	8243,26	524,35	7544,60	523,05	7683,22
525,60	8191,86	524,30	7858,33	523	7587,27
525,55	8220,23	524,25	7676,12	522,95	7530,41
525,50	8008,73	524,20	7612,38	522,90	7555,07
525,45	7985,65	524,15	7577,83	522,85	7524,46
525,40	7916,01	524,10	7576,49	522,80	7575,82
525,35	7890,25	524,05	7678,21	522,75	7636,26
525,30	7785,62	524	7758,87	522,70	7788,63
525,25	7865,14	523,95	7715,99	522,65	7614,75
525,20	7959,21	523,90	7615,43	522,60	7727,13
525,15	7919,15	523,85	7550,18	522,55	7544,03
525,10	7726,35	523,80	7571,24	522,50	7683,30
525,05	7834,18	523,75	7530,50	522,45	7617,71
525	7834,61	523,70	7591,69	522,40	7530,78
524,95	7862,58	523,65	7687,46	522,35	7600,32
524,90	7719,93	523,60	7710,21	522,30	7600,86
524,85	7706,67	523,55	7669,09	522,25	7670,99
524,80	7799,37	523,50	7739,75	522,20	7630,48
524,75	7750,11	523,45	7528,61	522,15	7685,69
524,70	7631,83	523,40	7653,61	522,10	7688,47
524,65	7768,27	523,35	7622,07	522,05	7604,71
524,60	7745,27	523,30	7727,62	522	7616,48
524,55	7766,97	523,25	7746,67		
524,50	7492,36	523,20	7497,72		

Fe 2p

1000 eV

740	16316,50	738,40	16421,50	736,80	16360,10
739,90	16334,50	738,30	16375,90	736,70	16388,70
739,80	16231	738,20	16366	736,60	16321,50
739,70	16257,70	738,10	16203,70	736,50	16300
739,60	16361,30	738	16206,10	736,40	16292,10
739,50	16388,20	737,90	16286,70	736,30	16407,70
739,40	16345,80	737,80	16438,10	736,20	16438,80
739,30	16199,60	737,70	16408,30	736,10	16236,10
739,20	16271	737,60	16199,20	736	16351,40
739,10	16357,30	737,50	16271,70	735,90	16406,30
739	16363	737,40	16096,30	735,80	16518,40
738,90	16422,90	737,30	16221,50	735,70	16406,30
738,80	16306	737,20	16268,90	735,60	16157
738,70	16293	737,10	16260,50	735,50	16242,10
738,60	16446,40	737	16320,10	735,40	16347,20
738,50	16350,60	736,90	16353,80	735,30	16261,80

735,20	16383,80	730,50	16128,90	725,80	16239,40
735,10	16285,60	730,40	16115,10	725,70	16056,90
735	16270,90	730,30	16163,50	725,60	16152,10
734,90	16273,70	730,20	16089,10	725,50	16367,80
734,80	16458	730,10	16102,10	725,40	16192
734,70	16264,90	730	16290,50	725,30	16251,60
734,60	16012,10	729,90	16352,70	725,20	16177,50
734,50	16132,50	729,80	16185,70	725,10	16141,80
734,40	16228,60	729,70	16244,70	725	16248,50
734,30	16306,80	729,60	16208,50	724,90	16249,90
734,20	16288,90	729,50	16131,50	724,80	16377,70
734,10	16309,10	729,40	16023,70	724,70	16250,10
734	16342,60	729,30	15953,50	724,60	16381,10
733,90	16406	729,20	16034	724,50	16201,30
733,80	16111,90	729,10	16301	724,40	16202,10
733,70	16160,40	729	16308	724,30	16393,10
733,60	16309,10	728,90	16065,60	724,20	16256,80
733,50	16360	728,80	16125	724,10	16079,40
733,40	16305,30	728,70	15979,10	724	16134,10
733,30	16371,60	728,60	16023,40	723,90	16142,20
733,20	16211,60	728,50	16018,80	723,80	16152,70
733,10	16113,80	728,40	16105,30	723,70	16260,70
733	16217,50	728,30	16289,60	723,60	16128,80
732,90	16434,20	728,20	16222,90	723,50	16399,40
732,80	16301,40	728,10	16204,20	723,40	16476,40
732,70	16115,30	728	16299,50	723,30	16318,10
732,60	16245,10	727,90	16192,10	723,20	16232
732,50	16248,20	727,80	16238,40	723,10	16211,20
732,40	16139,80	727,70	16205,60	723	16324,90
732,30	16198,90	727,60	16194,80	722,90	16279,10
732,20	16179,80	727,50	16270,80	722,80	16409,40
732,10	16220,10	727,40	16245,40	722,70	16426,30
732	16035	727,30	16252,90	722,60	16460,70
731,90	16224,90	727,20	16234,80	722,50	16523,60
731,80	16126,80	727,10	16117	722,40	16495,70
731,70	16171,90	727	16214,10	722,30	16477
731,60	16282	726,90	16356	722,20	16539,30
731,50	16277,20	726,80	16355,90	722,10	16528,30
731,40	16386,20	726,70	16167,10	722	16494,10
731,30	16369,50	726,60	16233,10	721,90	16655
731,20	16147	726,50	16182,10	721,80	16534,90
731,10	16324,20	726,40	16350,90	721,70	16462,30
731	16252,60	726,30	16351,40	721,60	16462,30
730,90	16149,80	726,20	16089,20	721,50	16656,10
730,80	16198,60	726,10	16066,90	721,40	16672,80
730,70	15980,10	726	16159	721,30	16923,10
730,60	16083,30	725,90	16237	721,20	16728

721,10	16522,10	716,40	15668	711,70	15968,10
721	16379,10	716,30	15693,50	711,60	15798,50
720,90	16567,10	716,20	15670,50	711,50	16016
720,80	16649,90	716,10	15709	711,40	15906
720,70	16593,30	716	15609,50	711,30	15971,30
720,60	16876,70	715,90	15659	711,20	15904,30
720,50	16726,60	715,80	15625,10	711,10	15804,90
720,40	16572,80	715,70	15474,60	711	16043,40
720,30	16652	715,60	15413,10	710,90	15975,60
720,20	16724,90	715,50	15597,10	710,80	15947,80
720,10	16584,30	715,40	15663,80	710,70	15888,90
720	16451,60	715,30	15649,40	710,60	16006,30
719,90	16597,50	715,20	15618,10	710,50	15909
719,80	16429,60	715,10	15435,10	710,40	15998,30
719,70	16496,60	715	15286,50	710,30	15825,90
719,60	16312,30	714,90	15401,40	710,20	15989,40
719,50	16504,70	714,80	15429,50	710,10	16091,80
719,40	16335,50	714,70	15428,10	710	16221,30
719,30	16085,30	714,60	15660,50	709,90	16334,70
719,20	16307,30	714,50	15418,60	709,80	16394,10
719,10	16236,60	714,40	15598,10	709,70	16287,60
719	16265,10	714,30	15606,40	709,60	16395,70
718,90	16207,90	714,20	15458,30	709,50	16477,10
718,80	16204,20	714,10	15576	709,40	16445,80
718,70	16204,20	714	15440,10	709,30	16498,80
718,60	16079	713,90	15565	709,20	16567,70
718,50	16014,50	713,80	15606,60	709,10	16733,10
718,40	15906	713,70	15368,70	709	16680,60
718,30	16035,70	713,60	15420,10	708,90	16790,70
718,20	16026,40	713,50	15700,80	708,80	16906,40
718,10	15998,80	713,40	15776,40	708,70	16678,20
718	16008,20	713,30	15658,70	708,60	16683,40
717,90	16136,90	713,20	15682,60	708,50	16989,20
717,80	16003,40	713,10	15553,90	708,40	16928,80
717,70	15889,50	713	15733,80	708,30	16896,70
717,60	16089,60	712,90	15815,10	708,20	17055,30
717,50	16030,30	712,80	15773,20	708,10	17056,50
717,40	16053,90	712,70	15639,60	708	17042,90
717,30	15984,20	712,60	15581,30	707,90	17138,20
717,20	16154,50	712,50	15745	707,80	17182,50
717,10	16030,40	712,40	15808,60	707,70	17203,50
717	16049,40	712,30	15881,60	707,60	17222
716,90	16128,10	712,20	15691,10	707,50	17086,60
716,80	15937,70	712,10	15781,30	707,40	17304,60
716,70	16053,20	712	15844,40	707,30	17194,70
716,60	15922,70	711,90	15829,30	707,20	17005,80
716,50	15774,40	711,80	15699,10	707,10	17248,30

707	17119,30	704,60	15701,40	702,20	13870,60
706,90	17160,50	704,50	15773,50	702,10	13733,60
706,80	16976,70	704,40	15919,80	702	13598,40
706,70	16849,50	704,30	15645,90	701,90	13595,20
706,60	17040,80	704,20	15664,60	701,80	13771,70
706,50	16802,50	704,10	15646,10	701,70	13808,30
706,40	16843,10	704	15485,40	701,60	13907,30
706,30	16766,70	703,90	15515,60	701,50	13773,90
706,20	16742,90	703,80	15196,60	701,40	13893,20
706,10	16811,80	703,70	14989,80	701,30	13675,40
706	16625,80	703,60	14960,30	701,20	13587,10
705,90	16419,20	703,50	14799,70	701,10	13589
705,80	16169,10	703,40	14738,40	701	13813,90
705,70	16129	703,30	14683,50	700,90	13816,90
705,60	16254,70	703,20	14262,90	700,80	13735,70
705,50	16079,70	703,10	14417,40	700,70	13519,20
705,40	16033,30	703	14240,50	700,60	13621,30
705,30	15879,30	702,90	14112,10	700,50	13580,10
705,20	15880,70	702,80	14130,10	700,40	13741,80
705,10	15872,70	702,70	14010,20	700,30	13784,80
705	15791,40	702,60	13889,20	700,20	13652,70
704,90	15740,10	702,50	13802,10	700,10	14033,80
704,80	15668	702,40	13878,90	700	13771,30
704,70	15750,10	702,30	13652,70		

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590	16944,80	588,40	17256,70	586,80	17607,60
589,90	17014,90	588,30	17092,60	586,70	17702,70
589,80	16906,30	588,20	17192,10	586,60	17631,70
589,70	16946	588,10	17174,10	586,50	17781
589,60	16871,40	588	17261,50	586,40	17683,80
589,50	17195,40	587,90	17256	586,30	17920,50
589,40	17067,60	587,80	17413,80	586,20	18111,10
589,30	17204,80	587,70	17368,40	586,10	17962,10
589,20	17113	587,60	17491,70	586	17881,80
589,10	17217,80	587,50	17354	585,90	18149,10
589	17149,60	587,40	17569,80	585,80	18272,10
588,90	17181,70	587,30	17419,80	585,70	18153,80
588,80	17177,20	587,20	17569,50	585,60	18303,70
588,70	17176,50	587,10	17519	585,50	18468,80
588,60	17187	587	17629,70	585,40	18423,30
588,50	17334,20	586,90	17473	585,30	18844,70

585,20	18725,60	580,50	17695,20	575,80	18698,30
585,10	18711,90	580,40	17546	575,70	19110,90
585	18948,60	580,30	17540,90	575,60	19360,50
584,90	19036,60	580,20	17510,80	575,50	19351,90
584,80	19231,50	580,10	17491,50	575,40	19501,10
584,70	19239,80	580	17351,20	575,30	19866,30
584,60	19538,10	579,90	17407,90	575,20	20068,30
584,50	19357	579,80	17379,50	575,10	20106,90
584,40	19446,90	579,70	17407,60	575	20329,10
584,30	19776,40	579,60	17333,60	574,90	20656,50
584,20	19600,20	579,50	17230,20	574,80	20813,30
584,10	19537	579,40	17259,20	574,70	20931,60
584	19799,90	579,30	17189,10	574,60	21247,30
583,90	19958,80	579,20	17228,80	574,50	21296,70
583,80	19942,60	579,10	17221,10	574,40	21436,20
583,70	19891,40	579	17206,20	574,30	21367,90
583,60	20009,90	578,90	17016,30	574,20	21397,70
583,50	19946,30	578,80	16992,10	574,10	21551,50
583,40	19630,60	578,70	17167,10	574	21888,60
583,30	19703,90	578,60	16987,20	573,90	21799,50
583,20	19811,40	578,50	17200,80	573,80	21607,20
583,10	19692,70	578,40	17351	573,70	21692,10
583	19629,30	578,30	17191,10	573,60	21672,40
582,90	19655,40	578,20	17262,90	573,50	21469,40
582,80	19302,10	578,10	17292,10	573,40	21413,40
582,70	19148	578	17124,20	573,30	21131,70
582,60	18818,80	577,90	17167,10	573,20	20994
582,50	18889,30	577,80	17211,60	573,10	20708,90
582,40	18806,10	577,70	17072	573	20697,70
582,30	18709,40	577,60	17315,10	572,90	20096,60
582,20	18781,50	577,50	17471,10	572,80	19933,20
582,10	18717,60	577,40	17411,20	572,70	19793,80
582	18517,90	577,30	17341,30	572,60	19572,50
581,90	18462	577,20	17455,80	572,50	19394,40
581,80	18327	577,10	17412,60	572,40	18918,30
581,70	18079,90	577	17569,20	572,30	18662,80
581,60	17958,60	576,90	17642	572,20	18589,50
581,50	18052,20	576,80	17708,20	572,10	18228
581,40	18014,60	576,70	17817	572	18072
581,30	18132	576,60	17903,20	571,90	17800
581,20	17915,80	576,50	17962,80	571,80	17875,20
581,10	17730,30	576,40	18076,20	571,70	17720,40
581	17698,70	576,30	18166,70	571,60	17773,10
580,90	17765	576,20	18397,20	571,50	17531,10
580,80	17756,30	576,10	18524,70	571,40	17340,80
580,70	17782,60	576	18662,70	571,30	17261,40
580,60	17850,30	575,90	18744,80	571,20	17152,20

571,10	17107	569	15625,30	566,90	15424,30
571	17055,70	568,90	15389,80	566,80	15598,20
570,90	17007,30	568,80	15599,60	566,70	15518,90
570,80	16665,10	568,70	15583,90	566,60	15617,10
570,70	16712	568,60	15368,10	566,50	15449,40
570,60	16580,60	568,50	15365,90	566,40	15278,90
570,50	16656,50	568,40	15451,90	566,30	15392,70
570,40	16390,30	568,30	15437,60	566,20	15555,30
570,30	16218	568,20	15434,20	566,10	15407,40
570,20	15938,80	568,10	15472,10	566	15373,80
570,10	15919,70	568	15404,70	565,90	15351,50
570	15898,10	567,90	15486,30	565,80	15397,60
569,90	15898,60	567,80	15281,50	565,70	15553,90
569,80	15839	567,70	15499,90	565,60	15496,60
569,70	15767,40	567,60	15678	565,50	15570,50
569,60	15547,80	567,50	15562,60	565,40	15455,30
569,50	15430,40	567,40	15526,10	565,30	15376,20
569,40	15657,90	567,30	15564,20	565,20	15392,60
569,30	15458,20	567,20	15514,90	565,10	15433,80
569,20	15510,70	567,10	15452,80	565	15682,30
569,10	15629,60	567	15480		

Cl 2p

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202	2988,86	201,20	3027,51	200,40	3116,65
201,95	3049,17	201,15	3043,08	200,35	3101,86
201,90	3031,68	201,10	3160,84	200,30	3102,65
201,85	2987,96	201,05	3151,54	200,25	3110,69
201,80	3164,39	201	3165,89	200,20	3154,96
201,75	3113	200,95	3166,91	200,15	3080,94
201,70	2996,12	200,90	3124,29	200,10	3034,01
201,65	2986,81	200,85	3117,58	200,05	3165,14
201,60	3064,70	200,80	3131,41	200	3168,79
201,55	2980,69	200,75	3188,13	199,95	3148,44
201,50	3095,75	200,70	3120,12	199,90	3055,08
201,45	3052,81	200,65	3057,90	199,85	3070,83
201,40	3094,44	200,60	3078,47	199,80	3098,50
201,35	3092,94	200,55	3016,11	199,75	3138,90
201,30	3145,82	200,50	3115,98	199,70	3108,41
201,25	3088,18	200,45	3146,68	199,65	3164,87

199,60	3148,09	197,25	3907,72	194,90	3696,07
199,55	3065,43	197,20	3847,48	194,85	3712,44
199,50	3049,61	197,15	3929,02	194,80	3629,95
199,45	3119,67	197,10	3999,52	194,75	3632,89
199,40	3141,21	197,05	3929,45	194,70	3550,98
199,35	3199,45	197	3953,93	194,65	3557,38
199,30	3145,50	196,95	4002,42	194,60	3527,72
199,25	3156,55	196,90	4004,38	194,55	3457,54
199,20	3274,96	196,85	4000,22	194,50	3406,27
199,15	3210,59	196,80	4002,94	194,45	3333,14
199,10	3250,71	196,75	4029,85	194,40	3338,38
199,05	3248,75	196,70	3993,88	194,35	3269,71
199	3140,85	196,65	4033,77	194,30	3270,51
198,95	3215,05	196,60	4084,44	194,25	3252,59
198,90	3237,37	196,55	4092,94	194,20	3206,24
198,85	3252,52	196,50	4081,72	194,15	3226,29
198,80	3153,22	196,45	4059,32	194,10	3191,08
198,75	3277,49	196,40	4140,72	194,05	3119,98
198,70	3252,86	196,35	4148,58	194	3212,65
198,65	3303,54	196,30	4233,56	193,95	3113,88
198,60	3325,74	196,25	4091,38	193,90	3118,84
198,55	3331,39	196,20	4168,86	193,85	3151,97
198,50	3395,62	196,15	4185,08	193,80	3147,29
198,45	3428,23	196,10	4205,15	193,75	3203,73
198,40	3405,99	196,05	4247,19	193,70	3185,78
198,35	3431,05	196	4319,63	193,65	3059,74
198,30	3404,03	195,95	4300,48	193,60	3042,85
198,25	3396,41	195,90	4227,15	193,55	3098,33
198,20	3525,91	195,85	4278,01	193,50	3126,27
198,15	3532,84	195,80	4296,38	193,45	3104,86
198,10	3580,75	195,75	4305,99	193,40	3116,38
198,05	3614,29	195,70	4335,55	193,35	3131,71
198	3611,53	195,65	4369,59	193,30	3151,29
197,95	3575,75	195,60	4305,92	193,25	3098,37
197,90	3640,50	195,55	4167,65	193,20	3120,43
197,85	3589,05	195,50	4258,51	193,15	3097,14
197,80	3633,62	195,45	4167,85	193,10	3075,14
197,75	3693,60	195,40	4170,83	193,05	3047,72
197,70	3734,94	195,35	4149,58	193	3048,52
197,65	3705,17	195,30	4159,39	192,95	3052,45
197,60	3733,60	195,25	4081,20	192,90	3096,29
197,55	3771,28	195,20	3963,29	192,85	3026,57
197,50	3756,34	195,15	3975,25	192,80	3065,42
197,45	3845,93	195,10	4002,70	192,75	2987,21
197,40	3761,68	195,05	3925,89	192,70	3035,85
197,35	3748,16	195	3789,32	192,65	3035,50
197,30	3744,41	194,95	3722,79	192,60	3057,04

192,55	3049,60	191,65	3085,22	190,75	3068,95
192,50	3067,21	191,60	3114,27	190,70	3083,98
192,45	3055,55	191,55	3080,72	190,65	3069,30
192,40	3030,51	191,50	3045,46	190,60	3037,14
192,35	2980,24	191,45	3131,22	190,55	3131,33
192,30	3079,02	191,40	3096,23	190,50	2994,91
192,25	3009,62	191,35	3036,77	190,45	3065,37
192,20	3043,40	191,30	3046,71	190,40	3090,73
192,15	3060,37	191,25	3030,20	190,35	3090,45
192,10	3076,09	191,20	3007,83	190,30	3140,73
192,05	3039,83	191,15	3052,74	190,25	3016,25
192	2977,81	191,10	3123,73	190,20	3009,50
191,95	2967,04	191,05	3070,56	190,15	3108,95
191,90	3117,25	191	2982,57	190,10	3119,66
191,85	3016,40	190,95	3054,29	190,05	3100,12
191,80	3040,03	190,90	3084,08	190	3109,18
191,75	3072,48	190,85	3072,08		
191,70	3133,42	190,80	3127,61		

Fe 2p
760 eV

		737,80	369007	735,50	282590
740	493667	737,70	364333	735,40	279795
739,90	487443	737,60	360346	735,30	276605
739,80	481680	737,50	354841	735,20	274158
739,70	476438	737,40	350901	735,10	271212
739,60	468434	737,30	346854	735	267844
739,50	462252	737,20	342521	734,90	265298
739,40	455649	737,10	338883	734,80	262106
739,30	449361	737	334910	734,70	259614
739,20	443225	736,90	330901	734,60	256962
739,10	437744	736,80	327104	734,50	254182
739	432291	736,70	323184	734,40	251724
738,90	426226	736,60	319318	734,30	249424
738,80	420028	736,50	315469	734,20	246109
738,70	414678	736,40	312309	734,10	243628
738,60	409247	736,30	308807	734	242199
738,50	404050	736,20	305232	733,90	238967
738,40	397966	736,10	301846	733,80	237427
738,30	393073	736	298566	733,70	236164
738,20	389082	735,90	295159	733,60	232824
738,10	383356	735,80	291667	733,50	230276
738	379497	735,70	289171	733,40	228361
737,90	374406	735,60	285476	733,30	226380

733,20	223641	728,50	151977	723,80	110908
733,10	221620	728,40	151117	723,70	110131
733	220659	728,30	149733	723,60	109757
732,90	218429	728,20	148149	723,50	108967
732,80	215951	728,10	147537	723,40	108443
732,70	213598	728	146465	723,30	107772
732,60	211609	727,90	145437	723,20	106666
732,50	209736	727,80	144284	723,10	106222
732,40	208195	727,70	143548	723	105606
732,30	206986	727,60	142616	722,90	105011
732,20	204410	727,50	141610	722,80	104331
732,10	202512	727,40	140929	722,70	103237
732	201168	727,30	139752	722,60	102966
731,90	198945	727,20	138568	722,50	102981
731,80	196980	727,10	137761	722,40	101930
731,70	195389	727	136220	722,30	101424
731,60	194180	726,90	134942	722,20	100920
731,50	192694	726,80	134137	722,10	100327
731,40	191127	726,70	133781	722	99517
731,30	188503	726,60	133517	721,90	99274,40
731,20	187713	726,50	131897	721,80	98368,50
731,10	185826	726,40	130794	721,70	98207
731	184313	726,30	130183	721,60	97234,20
730,90	182421	726,20	129056	721,50	97047,70
730,80	181955	726,10	128199	721,40	96885
730,70	180043	726	128301	721,30	95344,40
730,60	178828	725,90	127141	721,20	94657,20
730,50	176996	725,80	126003	721,10	93931,10
730,40	176133	725,70	125464	721	94065,40
730,30	174450	725,60	124346	720,90	93471,90
730,20	173465	725,50	123192	720,80	92669
730,10	171650	725,40	122883	720,70	91928,40
730	169944	725,30	121426	720,60	91731,80
729,90	168189	725,20	120875	720,50	90948,20
729,80	167705	725,10	120329	720,40	90334,10
729,70	166038	725	119916	720,30	89962,50
729,60	165040	724,90	119050	720,20	89320,70
729,50	163382	724,80	117937	720,10	88635
729,40	162055	724,70	117201	720	88773
729,30	161041	724,60	116235	719,90	87974
729,20	160175	724,50	115504	719,80	87415,70
729,10	159009	724,40	115354	719,70	86467,40
729	157401	724,30	114410	719,60	86245,90
728,90	156310	724,20	113762	719,50	85730,20
728,80	155270	724,10	113057	719,40	85047,20
728,70	154318	724	112182	719,30	84908,10
728,60	153225	723,90	110824	719,20	84695,70

719,10	83719,30	714,40	67658,20	709,70	55751,50
719	83363,70	714,30	67653,90	709,60	55391,20
718,90	83297	714,20	66859,40	709,50	55546,50
718,80	82745,50	714,10	66659,10	709,40	55310
718,70	82084,90	714	66743,90	709,30	55117,10
718,60	82083,40	713,90	66236,80	709,20	54763
718,50	81630,20	713,80	66331,50	709,10	54482,60
718,40	81378,90	713,70	65645,10	709	54299,90
718,30	81076,90	713,60	65121,50	708,90	54010,30
718,20	80575,80	713,50	65268,20	708,80	53965
718,10	79930	713,40	64981,70	708,70	53630,40
718	79213,80	713,30	64438,50	708,60	53393,70
717,90	79083,10	713,20	64562,80	708,50	53025,70
717,80	78888,50	713,10	63999,40	708,40	53028,20
717,70	78300,10	713	63943,30	708,30	53010,70
717,60	78205,70	712,90	63705,10	708,20	52717,10
717,50	78124,80	712,80	63181,90	708,10	52497,70
717,40	77561,70	712,70	62514,80	708	51759,80
717,30	77100,50	712,60	62508,50	707,90	51679
717,20	76945,50	712,50	62441,20	707,80	51181,40
717,10	76347,30	712,40	61908	707,70	51274,10
717	76259,70	712,30	61637,60	707,60	51129,10
716,90	75760,40	712,20	61653,60	707,50	50555,90
716,80	74995,40	712,10	61444,30	707,40	50158,90
716,70	74410,50	712	60893,70	707,30	49988,40
716,60	74656,40	711,90	60643,30	707,20	49592,90
716,50	74542,70	711,80	60486,90	707,10	49343,10
716,40	73929,30	711,70	60382	707	48644,90
716,30	73055,20	711,60	59700,40	706,90	48365,40
716,20	73299	711,50	59574,30	706,80	47909,40
716,10	72981,40	711,40	59428,70	706,70	47639,70
716	72221,40	711,30	59140,80	706,60	47746,60
715,90	71933,80	711,20	59104,70	706,50	47595,30
715,80	71657	711,10	58477,40	706,40	47190,50
715,70	71246,70	711	58427,10	706,30	46854,40
715,60	71168,90	710,90	58329,60	706,20	46338,90
715,50	70548,80	710,80	58317,10	706,10	46178
715,40	70627,10	710,70	58115,60	706	45838,50
715,30	69931,10	710,60	57663,70	705,90	45624,50
715,20	69868,50	710,50	57561,10	705,80	45327,20
715,10	69475,30	710,40	57068,70	705,70	45183,80
715	69315	710,30	56830,30	705,60	44636,80
714,90	69305,70	710,20	56854,20	705,50	44793,20
714,80	68839,90	710,10	56414,40	705,40	44479,30
714,70	68317,70	710	56391,30	705,30	44515,10
714,60	68505,80	709,90	56030,20	705,20	44034,90
714,50	67737,30	709,80	55846,30	705,10	44103,20

705	43578,30	703,30	40946,20	701,60	38539,50
704,90	43297,40	703,20	40701,90	701,50	38393,60
704,80	43612	703,10	40501,40	701,40	38501,30
704,70	43328,60	703	40464,60	701,30	38445,50
704,60	43293,30	702,90	40270,80	701,20	38269,40
704,50	43027,70	702,80	40080,60	701,10	37975,50
704,40	42631,30	702,70	40262,30	701	37779,90
704,30	42339,20	702,60	40149,40	700,90	37507
704,20	42190,10	702,50	39723,10	700,80	37649,80
704,10	42014,40	702,40	39346,40	700,70	37439,50
704	42118,70	702,30	39412,90	700,60	37704
703,90	41989,90	702,20	39486,30	700,50	37204,80
703,80	41896,90	702,10	39276,90	700,40	37134
703,70	41264,60	702	39255,20	700,30	36891,40
703,60	41552,90	701,90	39199,40	700,20	37078,60
703,50	41351,30	701,80	39127,40	700,10	36902
703,40	41260,80	701,70	38844,20	700	36663,90

Cr 2p

630 eV

600	13025,60	597,80	11118,90	595,60	9700,35
599,90	12830,50	597,70	10999,10	595,50	9668,21
599,80	12884,20	597,60	11115,70	595,40	9601,71
599,70	12784,80	597,50	11016,80	595,30	9612,32
599,60	12850,80	597,40	10945,50	595,20	9438,01
599,50	12783,70	597,30	10859,30	595,10	9273,98
599,40	12605,30	597,20	10741,70	595	9290,36
599,30	12410,90	597,10	10725	594,90	9251,58
599,20	12371	597	10728,80	594,80	9290,01
599,10	12117,60	596,90	10684,70	594,70	9142,99
599	12105,60	596,80	10400,30	594,60	9170,64
598,90	12045,30	596,70	10267,50	594,50	9046,69
598,80	11988,30	596,60	10242,80	594,40	8880,69
598,70	11767,20	596,50	10138,40	594,30	8835,39
598,60	11703,70	596,40	10128,40	594,20	8657,21
598,50	11728,50	596,30	10028,50	594,10	8878,31
598,40	11700,60	596,20	9970,76	594	8679,23
598,30	11573,70	596,10	10064,30	593,90	8554,92
598,20	11363,70	596	10011	593,80	8490,72
598,10	11432,40	595,90	9961,15	593,70	8407,84
598	11408,90	595,80	9831,19	593,60	8364,44
597,90	11300,40	595,70	9657,10	593,50	8340,81

593,40	8319,70	588,70	6390,33	584	5257,58
593,30	8303,06	588,60	6529,27	583,90	5187,96
593,20	8258,15	588,50	6281,42	583,80	5096,58
593,10	8254,04	588,40	6335,72	583,70	5161,57
593	8268,84	588,30	6325,52	583,60	5169,61
592,90	8130,17	588,20	6187,31	583,50	4993,74
592,80	8137,96	588,10	6224,20	583,40	5009,94
592,70	8077,39	588	6298,01	583,30	5136,04
592,60	7815,03	587,90	6299,05	583,20	4972,75
592,50	7758,10	587,80	6261,18	583,10	4798,65
592,40	7802,49	587,70	6222,25	583	4847,92
592,30	7810,57	587,60	6187,77	582,90	4801,48
592,20	7686,41	587,50	6218,69	582,80	4839,99
592,10	7736,81	587,40	6129,32	582,70	4775,92
592	7691	587,30	6141,39	582,60	4761,89
591,90	7633,10	587,20	6214,21	582,50	4733,19
591,80	7473,38	587,10	6092,12	582,40	4660,32
591,70	7480,82	587	6026,54	582,30	4638,38
591,60	7427	586,90	6050,86	582,20	4723,42
591,50	7427,02	586,80	6078,91	582,10	4642,27
591,40	7323,34	586,70	5922,69	582	4694,97
591,30	7258,96	586,60	5956,92	581,90	4626,60
591,20	7299,09	586,50	5872,11	581,80	4558,43
591,10	7267,92	586,40	5892,03	581,70	4565,99
591	7134,59	586,30	5903,18	581,60	4593,42
590,90	7154,19	586,20	5989,46	581,50	4455,34
590,80	7179,80	586,10	6025,18	581,40	4502,02
590,70	7024,87	586	5954,86	581,30	4532,46
590,60	7064,83	585,90	5981,62	581,20	4327,50
590,50	7087,34	585,80	5940,28	581,10	4312,56
590,40	6962,38	585,70	5786,90	581	4325,47
590,30	7101,08	585,60	5829,50	580,90	4359,22
590,20	6887,43	585,50	5885,70	580,80	4314,99
590,10	6735,92	585,40	5788,48	580,70	4212,80
590	6774,68	585,30	5782,96	580,60	4275,22
589,90	6825,73	585,20	5756,21	580,50	4342,72
589,80	6786,92	585,10	5807,59	580,40	4249,38
589,70	6831,45	585	5712,56	580,30	4308,47
589,60	6771,56	584,90	5726,95	580,20	4307,63
589,50	6666,27	584,80	5542,90	580,10	4198,55
589,40	6500,11	584,70	5447,03	580	4273,61
589,30	6528,56	584,60	5487,59	579,90	4312,27
589,20	6639,88	584,50	5497,45	579,80	4163,88
589,10	6499,92	584,40	5318,96	579,70	4119,96
589	6566,86	584,30	5349,24	579,60	4197,23
588,90	6409,50	584,20	5264,81	579,50	4128,58
588,80	6314,26	584,10	5240,42	579,40	4161,72

579,30	4114,99	574,60	3707,44	569,90	2805,77
579,20	4106,92	574,50	3648,54	569,80	2785,66
579,10	4124,86	574,40	3695,92	569,70	2834,76
579	4029,83	574,30	3609,50	569,60	2827,93
578,90	4164,71	574,20	3511,90	569,50	2832,82
578,80	4137,93	574,10	3430,28	569,40	2771,18
578,70	4087,30	574	3477,43	569,30	2814,90
578,60	4023,49	573,90	3406,04	569,20	2840,76
578,50	3998,04	573,80	3334,11	569,10	2804,51
578,40	3971,86	573,70	3315,59	569	2821,92
578,30	4090,54	573,60	3262,36	568,90	2843,45
578,20	4086,99	573,50	3243,81	568,80	2814,76
578,10	3944,66	573,40	3275,28	568,70	2779,89
578	4066,40	573,30	3206,52	568,60	2732,84
577,90	4126,11	573,20	3175,24	568,50	2750,98
577,80	4085,32	573,10	3125,63	568,40	2808,93
577,70	4079,67	573	3161,86	568,30	2766,85
577,60	4042,31	572,90	3126,53	568,20	2723,36
577,50	4071,51	572,80	3011,41	568,10	2693,42
577,40	4106,70	572,70	3082,67	568	2662,19
577,30	3998,78	572,60	3063,65	567,90	2670,72
577,20	3990,89	572,50	3120,72	567,80	2668,02
577,10	4092,75	572,40	3053,06	567,70	2700,54
577	4195,66	572,30	3035,84	567,60	2719,91
576,90	4097,19	572,20	3054,43	567,50	2634,05
576,80	4024,19	572,10	3027,78	567,40	2643,39
576,70	4151,71	572	3095,10	567,30	2704,97
576,60	4104,78	571,90	3036,78	567,20	2684,70
576,50	4066,14	571,80	2949,78	567,10	2666,12
576,40	4167,18	571,70	3060,96	567	2598,10
576,30	4124,51	571,60	3020,76	566,90	2601,96
576,20	4135,68	571,50	2959,48	566,80	2671,23
576,10	4038,70	571,40	2985,09	566,70	2641,36
576	4184,08	571,30	3010,15	566,60	2632,82
575,90	4134,64	571,20	2955,29	566,50	2590,87
575,80	4115,96	571,10	2973,22	566,40	2614,65
575,70	4162,12	571	2904,81	566,30	2631,84
575,60	4163,93	570,90	3012,26	566,20	2557,12
575,50	4116,48	570,80	2883,10	566,10	2551,84
575,40	4036,83	570,70	2856,27	566	2585,61
575,30	4095,25	570,60	2922,86	565,90	2576,35
575,20	3987,22	570,50	2862,73	565,80	2550,35
575,10	3943,51	570,40	2838,39	565,70	2552,37
575	3927,53	570,30	2917,15	565,60	2600,24
574,90	3953,27	570,20	2859,34	565,50	2576,90
574,80	3863,91	570,10	2869,63	565,40	2561,33
574,70	3789,27	570	2818,50	565,30	2606,48

565,20	2577,92	565,10	2578,03	565	2597,61

O 1s
580 eV

540	71977,50	536,10	58023,60	532,20	60331,30
539,90	71282,60	536	57949,40	532,10	61449,30
539,80	70983,50	535,90	57696,60	532	62154,80
539,70	70540,10	535,80	57610,90	531,90	63312,30
539,60	70230,80	535,70	57171,50	531,80	65092,80
539,50	70045	535,60	56976,80	531,70	66892,70
539,40	69694,80	535,50	56749	531,60	68647,60
539,30	69414	535,40	55986,70	531,50	70662,50
539,20	69226	535,30	55748,30	531,40	72195,70
539,10	68530,30	535,20	55673	531,30	73972,20
539	68022,10	535,10	55292,70	531,20	75971,50
538,90	67936,90	535	54625,20	531,10	77836,20
538,80	67206,90	534,90	54616	531	79493,30
538,70	66928,30	534,80	54501,50	530,90	80621,60
538,60	66775	534,70	54352,20	530,80	80819,50
538,50	66756,10	534,60	53958	530,70	80545,10
538,40	66174,50	534,50	54010,20	530,60	80280,20
538,30	65719,80	534,40	53363,60	530,50	79047,30
538,20	65135	534,30	53410,90	530,40	78010
538,10	65147,90	534,20	53243,90	530,30	76170,10
538	64644,50	534,10	53504,50	530,20	74027
537,90	64418,60	534	53420,20	530,10	72194,30
537,80	63914	533,90	52884,20	530	69842,90
537,70	63467,30	533,80	53265,40	529,90	67337
537,60	62966,10	533,70	53647,80	529,80	65561,30
537,50	62860,50	533,60	53539,10	529,70	63878,40
537,40	62601,90	533,50	53779,50	529,60	62030,40
537,30	62647,40	533,40	53841,80	529,50	60556
537,20	62066,80	533,30	53942,70	529,40	59525,80
537,10	61424,40	533,20	54111,40	529,30	58925,70
537	61408,20	533,10	54439,20	529,20	58357
536,90	61187,20	533	54717,20	529,10	57367,50
536,80	60850,10	532,90	55215,90	529	56445,50
536,70	60642,60	532,80	55832,70	528,90	54817,10
536,60	59939,90	532,70	56297,60	528,80	53785,10
536,50	59736,60	532,60	56705	528,70	52275,50
536,40	59145,20	532,50	57745,60	528,60	50356,40
536,30	58835,30	532,40	58488	528,50	48474,20
536,20	58141,30	532,30	59568	528,40	46557,20

528,30	44941,20	527,10	36980,60	525,90	35205,20
528,20	43269,70	527	37002,10	525,80	34914,30
528,10	42163,90	526,90	36769,80	525,70	34614,20
528	40917	526,80	36644,60	525,60	34487,40
527,90	39988,70	526,70	36235,30	525,50	34294,40
527,80	39229,30	526,60	36051,10	525,40	34431,70
527,70	38591,70	526,50	36085	525,30	34052
527,60	38403,80	526,40	35857,10	525,20	34127,80
527,50	38049,70	526,30	35701,70	525,10	33757,40
527,40	37744,30	526,20	35301,10	525	33875,30
527,30	37500,70	526,10	35577,30		
527,20	37297,80	526	35119		

Cl 2p

260 eV

205	1920,39	202,30	1688,16	199,60	2244,92
204,90	1940,45	202,20	1715,62	199,50	2217,98
204,80	1902,33	202,10	1792,01	199,40	2239,83
204,70	1868,83	202	1748,68	199,30	2173,82
204,60	1889,52	201,90	1730	199,20	2267,35
204,50	1902,92	201,80	1760,21	199,10	2339,57
204,40	1895,69	201,70	1800,89	199	2330,58
204,30	1893,12	201,60	1794,16	198,90	2433,62
204,20	1832,33	201,50	1765,66	198,80	2603,68
204,10	1787,82	201,40	1774,04	198,70	2562,82
204	1878,92	201,30	1824,53	198,60	2611,97
203,90	1805,60	201,20	1921,16	198,50	2621,44
203,80	1911,59	201,10	1918,92	198,40	2573,82
203,70	1858,66	201	1892,61	198,30	2627,69
203,60	1800,22	200,90	1924,97	198,20	2610,25
203,50	1802,97	200,80	2005,42	198,10	2509,34
203,40	1841,30	200,70	2047,96	198	2413,69
203,30	1863,96	200,60	2120,26	197,90	2329,18
203,20	1807,86	200,50	2164,14	197,80	2218,88
203,10	1801,40	200,40	2172,82	197,70	2065,90
203	1819,99	200,30	2206,60	197,60	1932,41
202,90	1775,29	200,20	2260,72	197,50	1913,73
202,80	1782,15	200,10	2261,16	197,40	1854,75
202,70	1746,24	200	2262,98	197,30	1782,57
202,60	1739,73	199,90	2257,11	197,20	1692,85
202,50	1741,63	199,80	2363,36	197,10	1627,25
202,40	1739,70	199,70	2281,14	197	1580,53

196,90	1554,64	196,20	1516,11	195,50	1472,50
196,80	1578,07	196,10	1507,75	195,40	1511,24
196,70	1620,26	196	1555,19	195,30	1489,91
196,60	1538,96	195,90	1483,03	195,20	1528,88
196,50	1527,26	195,80	1493,08	195,10	1508,74
196,40	1475,77	195,70	1515,10	195	1427,50
196,30	1508,39	195,60	1533,28		

S 2p
210 eV

175	514644	171,60	431671	168,20	405907
174,90	512760	171,50	429066	168,10	399782
174,80	510326	171,40	428665	168	392140
174,70	506845	171,30	427390	167,90	386831
174,60	503666	171,20	424775	167,80	381875
174,50	500018	171,10	424680	167,70	376927
174,40	497379	171	423382	167,60	373244
174,30	495049	170,90	423028	167,50	369599
174,20	491270	170,80	422094	167,40	367292
174,10	487800	170,70	422601	167,30	364903
174	484889	170,60	423194	167,20	362896
173,90	482993	170,50	423792	167,10	361135
173,80	479408	170,40	424048	167	359527
173,70	477573	170,30	423970	166,90	357782
173,60	474869	170,20	424922	166,80	356538
173,50	473259	170,10	424921	166,70	355350
173,40	470256	170	425841	166,60	353084
173,30	466997	169,90	425833	166,50	351012
173,20	465348	169,80	426537	166,40	349545
173,10	462926	169,70	425731	166,30	346710
173	460536	169,60	426824	166,20	346171
172,90	459437	169,50	426184	166,10	344767
172,80	456843	169,40	424437	166	342543
172,70	453901	169,30	424678	165,90	341631
172,60	450955	169,20	424753	165,80	339629
172,50	449422	169,10	425638	165,70	338208
172,40	446205	169	425865	165,60	336511
172,30	444711	168,90	426926	165,50	335588
172,20	443567	168,80	426519	165,40	334535
172,10	441531	168,70	425234	165,30	333258
172	439602	168,60	422841	165,20	332112
171,90	437904	168,50	420390	165,10	331597
171,80	434749	168,40	416515	165	330328
171,70	432030	168,30	411309		

Cr 3s
100 eV

79	1414690,00	76,60	1357020,00	74,20	976617
78,90	1403520,00	76,50	1351530,00	74,10	960084
78,80	1394320,00	76,40	1345930,00	74	941891
78,70	1387870,00	76,30	1338800,00	73,90	925465
78,60	1379900,00	76,20	1330220,00	73,80	911444
78,50	1374950,00	76,10	1319130,00	73,70	898623
78,40	1368660,00	76	1309610,00	73,60	886412
78,30	1363850,00	75,90	1299960,00	73,50	875831
78,20	1362630,00	75,80	1285680,00	73,40	866294
78,10	1360780,00	75,70	1272990,00	73,30	855679
78	1358220,00	75,60	1257710,00	73,20	848149
77,90	1359090,00	75,50	1241420,00	73,10	842271
77,80	1360050,00	75,40	1224520,00	73	834953
77,70	1362480,00	75,30	1208580,00	72,90	827571
77,60	1363120,00	75,20	1189010,00	72,80	821793
77,50	1365430,00	75,10	1169640,00	72,70	815426
77,40	1367070,00	75	1149580,00	72,60	808712
77,30	1368260,00	74,90	1128610,00	72,50	804358
77,20	1369500,00	74,80	1107830,00	72,40	800150
77,10	1369530,00	74,70	1085900,00	72,30	793693
77	1368390,00	74,60	1062660,00	72,20	789179
76,90	1367640,00	74,50	1041710,00	72,10	783940
76,80	1364120,00	74,40	1019640,00	72	779146
76,70	1359370,00	74,30	998202		