

An experimental high throughput to high fidelity study towards discovering Al-Cr containing corrosion-resistant compositionally complex alloys

SUPPLEMENTAL MATERIAL

Wavelength Dispersive Spectroscopy

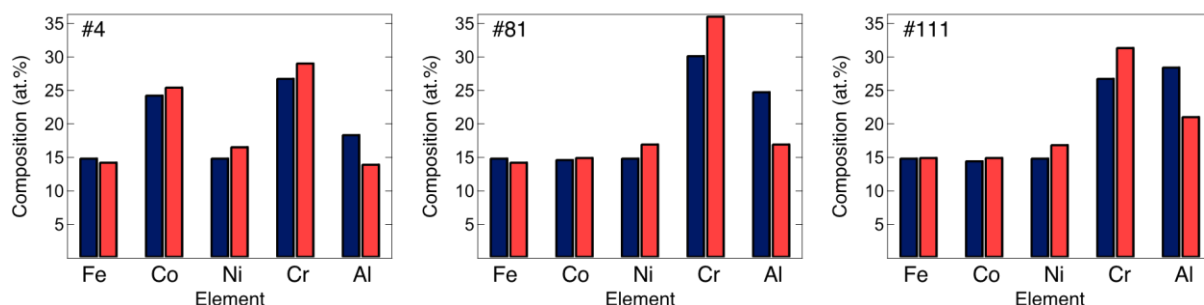


Fig. S1. Compositional information comparing the combi-alloy spots #4, #81 and #111. The dark-blue and red bars are the XRF and WDS data, respectively. The XRF data was measured using Bruker Tornado and analyzed using Crossroads XRD-MTFFP software. The WDS results were generated using an accelerating voltage of 15 kV and a beam current of 25 nA. All compositions provided in this figure are given in atomic percent.

Fig. S1 shows a comparison in Wavelength-Dispersive X-Ray Spectroscopy (WDS) and X-ray Fluorescence (XRF) data used for compositional analysis of waver samples #81-M, #4-O, and #111-O. The instrumentation and analyses methods used for XRF is described in the main text. For WDS, a JEOL-JXA 8530F field emission electron microprobe equipped with 5 wavelength-dispersive spectrometers. For all samples an accelerating voltage of 15 kV and a probe current of 25 nA with a 1 μm probe diameter was used for the quantitative analysis of Cr, Si, Al, Ni, Co, and Fe. The calibration standards used were pure metals of Si, Cr, Co, Ni, and Al, and counting times on the K α X-ray peaks of all elements analyzed were 30 seconds and 15 seconds on each background; this calibration yielded detection limits of 0.01 wt% for Si and Al, 0.02 wt% for Co, 0.03 wt% for Ni, and 0.04 wt% for Fe and Cr. To compensate for the overlap of the Fe K β X-ray peak with the Co K α X-ray peak, a correction was applied. Data acquisition and processing, including the application of the ZAF-correction algorithms of Pouchou and Pichoir [1] were performed, using the Probe for EPMA by Probe Software, Inc. To understand the excitation volume of the probe, the Monte Carlo simulation program McX-Ray was used where the depth of the X-ray excitation volume was modeled in a sample with a composition of 30 wt% Cr, 10 wt% Al, 20 wt% Co, 20 wt% Ni, and 20 wt% Fe for an accelerating voltage of 15 kV, a probe current of 25 nA and a probe diameter of 1 μm . Results of this simulation indicate the maximum depth of X-ray generation for this material is ca. 0.9 μm .

Scanning Electron Microscopy

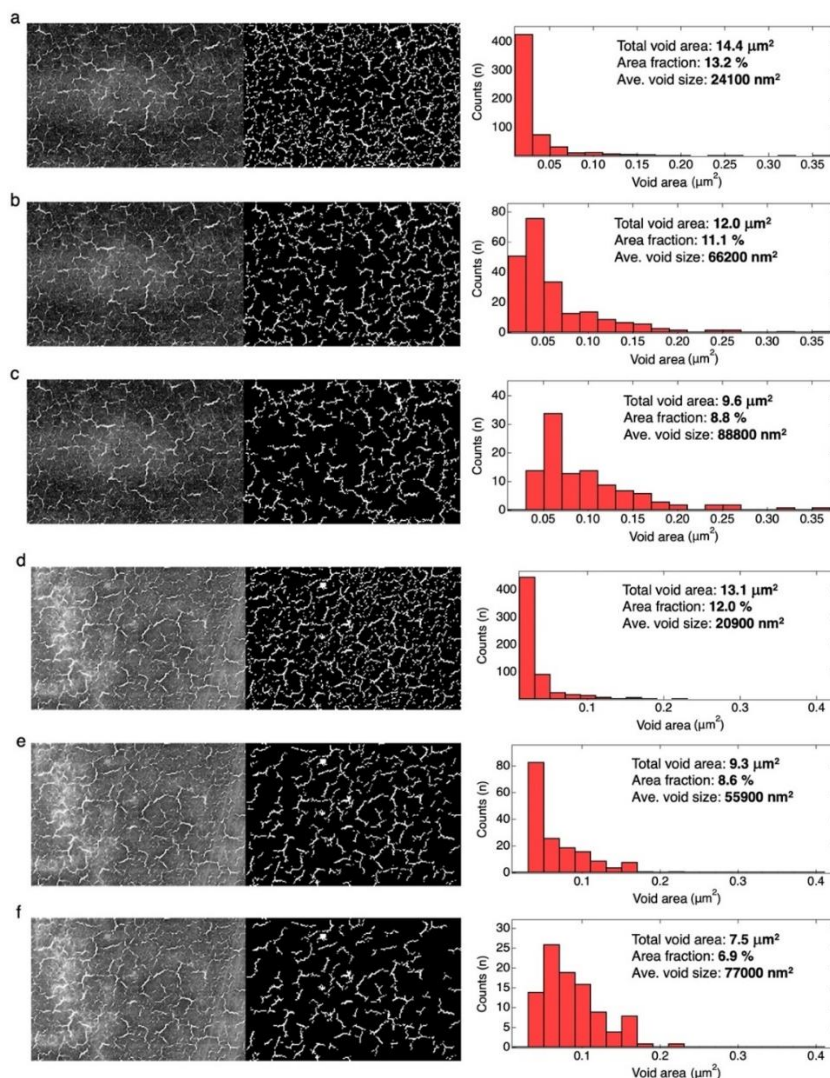


Fig. S2. Inverse greyscale and corresponding segmented images of the unexposed (**a-b-c**) and exposed (**d-e-f**) combi-wafer spot #81, with histograms of the void sizes across the surface. To highlight the range of possible differences in segmentation, a minimum pixel threshold of 4 (**a & d**), 24 (**b & e**) and 40 (**c & f**) are provided here. The values overlayed on the histograms represent the sum of void surface areas (total void area) and the percent of surface area those voids cover with respect to the total surface area of the image (area fraction).

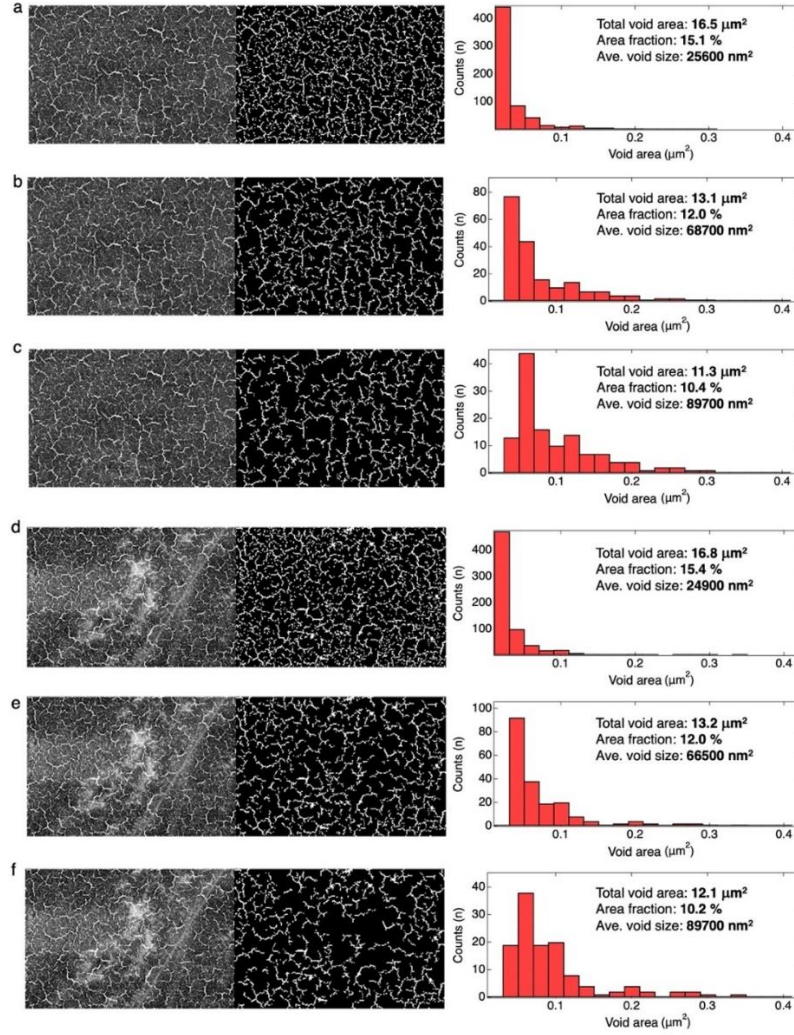


Fig. S3. Inverse greyscale and corresponding segmented images of the unexposed (**a-b-c**) and exposed (**d-e-f**) combi-wafer spot #36, with histograms of the void sizes across the surface. To highlight the range of possible differences in segmentation, a minimum pixel threshold of 4 (**a & d**), 24 (**b & e**) and 40 (**c & f**) are provided here. The values overlayed on the histograms represent the sum of void surface areas (total void area), the percent of surface area covered by those voids (area fraction) and the average void size (avg. void size).

SEM analysis of the exposed and unexposed wafer surfaces was performed using a Thermo Fisher Scientific Helios UC G4 scanning electron microscope (SEM) in secondary electron mode using a 20 kV accelerating voltage, beam current of 3.2 nA, and a dwell time of 1 μ s. The SEM images were then post-processed using a custom MATLAB code to determine the surface coverage and size of the voids across of the combi-film surface on wafer spots #81 and #36 (approximately 20 mm apart).[2]

Image analyses of #81 (**Fig. S2**) and #36 (**Fig. S3**) alloy surfaces were performed for three size thresholds of void selection: 4, 24, and 40 using a MATLAB code described elsewhere [2]. Segments were removed from consideration when the number of pixels that the segment consisted of fell below the threshold. Therefore, distributions skewed larger as minor cracks were filtered out. The largest difference observed remained below a 5% total area difference and between two fields of view varied by 2% thus, the differences were considered insignificant.

Pure Elements LSV and Linear Polarization Resistance

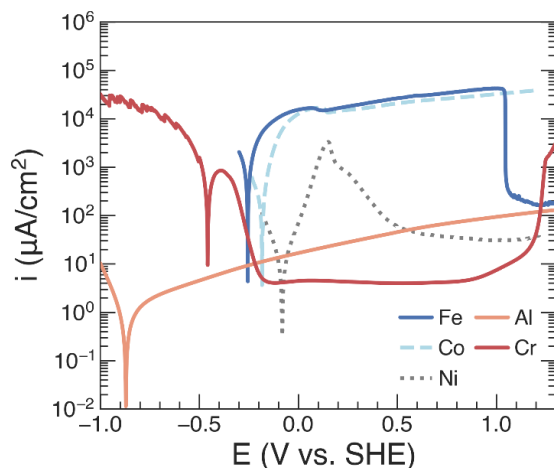


Fig. S4 Upward Linear Sweep Voltammetry of pure Al, Co, Cr, Fe and Ni at a scan rate of 1 mV/s in deaerated 0.1 mol/L H₂SO₄.

Fig. S4 shows the upward E-log(*i*) linear sweep voltammetry behavior of high purity Al, Cr, Fe, Co and Ni polished to 1 μm surface finish in deaerated 0.1 mol/L H₂SO₄. The anodic passivation behavior of the pure elements in the test media can help understand the role of elements played during passivation of a CCA containing these elements. The air formed oxides of these pure elements were cathodically cleaned by potentiostatically holding at -2.64 V (SHE) for 600s for Al and Cr, and -1 V (SHE) for 120 s for Fe, Co and Ni, respectively. Pure Al shows no active passive transition unlike Cr and forms a passive film at much lower anodic potentials. The passive current density of Cr is much lower than that of Al in the range from -0.2 V to above 1.0 V, suggesting that Al-Cr alloys its passive film more protective.

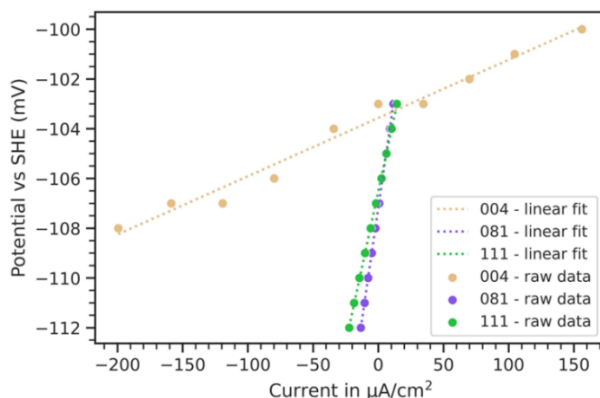


Fig. S5 Linear Polarization Resistance fitting of raw LSV data using 10 points across the corrosion potential of down selected alloys #4, #81 and #111.

Linear Polarization Resistance was determined following Scully [3], where 10 points just above and below the OCP in a normalized upward linear sweep voltammetry was taken to perform a linear fitting. The residuals of fit (R^2) were verified to be above 0.99. The slopes thus calculated were taken as the linear polarization resistance (LPR) of the individual alloy towards anodic dissolution. The linear fits for three down selected alloys for this study are shown in **Fig. S5**.

Scanning Transmission Electron Microscopy

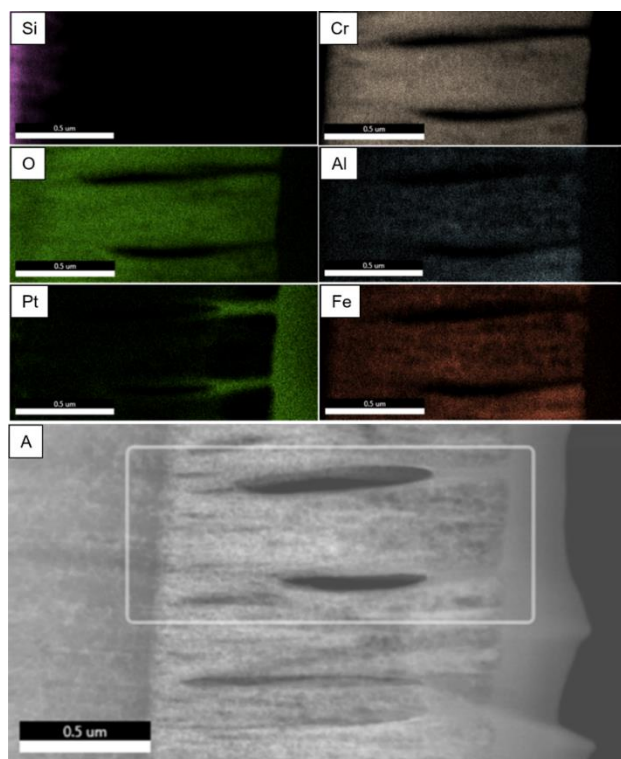


Fig. S6: Scanning Transmission Electron Microscopy elemental mapping with Energy Dispersive Spectroscopy (STEM-EDS) of Sample #4. Elemental distribution is largely homogeneous with some possible oxygen depletion observed near the surface of the film (white arrow).

STEM sample preparation with FIB proceeded as follows. Prior to ion beam milling, the sample surface was protected with platinum deposited with the electron beam until a platinum layer thickness of at least 500 nm was reached. An additional 2 μm of platinum was deposited using the ion beam to reach a total height of 2-3 μm. Samples were then attached to a copper STEM grid and thinned to ≈100 nm using the ion beam. The thinning was performed with a tilt of $\pm 3^\circ$, voltage of 16 kV followed by 8 kV, and with respective currents of 50 and 30 pA respectively. The final cleaning step was performed at 5 kV and 15 pA with a rotation of $\pm 1^\circ$.

Elemental analysis was performed via Electron Dispersive Spectroscopy (EDS) as part of the microstructural analysis via transmission electron microscopy (TEM). The EDS signal variations as shown in **Fig. S6** are suspected to originate from thickness variations as evidenced by a correlation in signal between differing elements instead of contrasting signal that may indicate local enrichment or depletion. Exceptions include a slight oxygen depletion at the surface on one side of the lower void that corresponds with an enrichment of alloying elements aluminum and iron. The film density thus adds signal variation to the elemental analysis that may be masking subtle elemental differences. The value of high-fidelity microstructural analysis can thus be improved by improving the film density.

STEM-EDS (Energy Dispersive Spectroscopy) of the wafer cross-sections suggests that the matrix of the wafer is chemically homogeneous in the #4, #81, and #111 as-corroded samples. The chromium is understood to be generally homogeneous as the oxygen map and corresponding transition metal maps have correlated dim regions where topography of the film may alter the signal intensity. Depletion of both

chromium and oxygen in the lower 100 nm of the film thickness corresponds to an enrichment in silicon from the substrate.

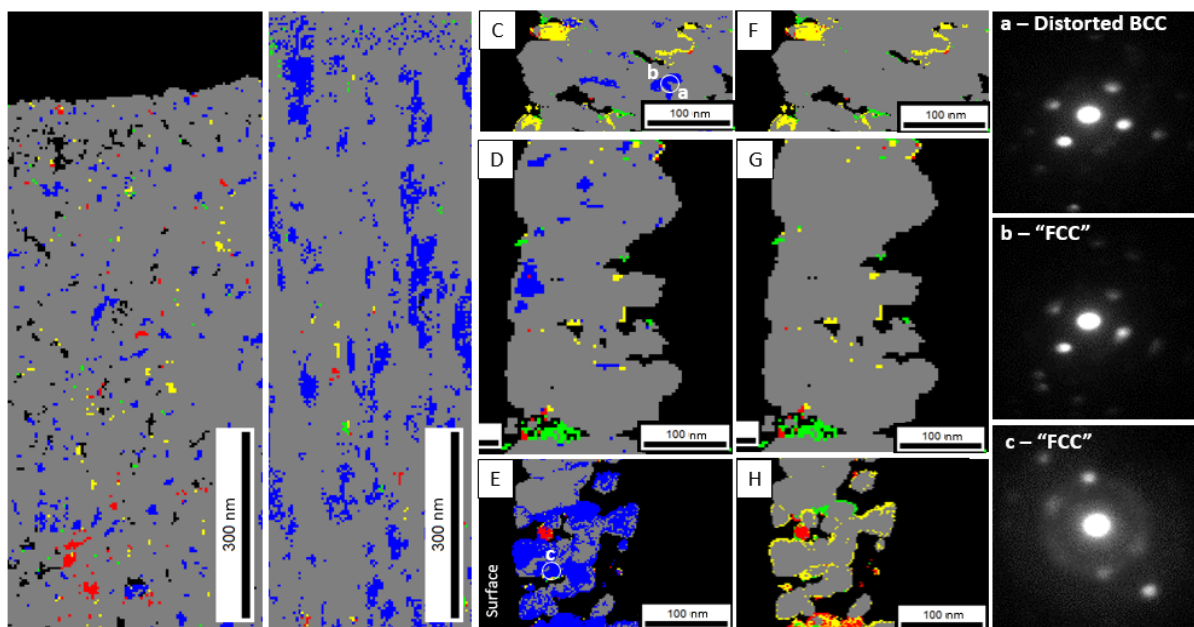


Fig. S7. PED indexing of (A & B) through-thickness PED map of #4 vs #111. Note that the FCC is only indexed to particular orientations in #111. It is probable that the distorted BCC structure is difficult to distinguish from FCC in that orientation. (C-F) PED maps of #81, #111, and #4, respectively, of the near-surface structure inclusive of an FCC reference in indexing. (G-H) PED maps of #81, #111, and #4, respectively, of the near-surface structure without the inclusion of an FCC reference.

A chromium iron FCC reference was used in the relative indexing of diffraction patterns via PED.

Table S1. Phase and grain size analysis from precession electron diffraction (PED) in the transmission electron microscope.

Stoichiometry	#Alloy	BCC (% Area)	FCC (% Area)	Al ₂ O ₃ (% Area)	Cr ₂ O ₃ (% Area)	Fe ₂ O ₃ (% Area)	Average Grain Diameter Manual (nm)	Average Grain Diameter OIM (nm)
Al _{0.28} Co _{0.15} Cr _{0.27} Fe _{0.15} Ni _{0.15}	111	93	4*	1	2	<1	30.3	14.7
Al _{0.25} Co _{0.15} Cr _{0.30} Fe _{0.15} Ni _{0.15}	81	90	4*	0	1	5	30.3	N/A
Al _{0.18} Co _{0.25} Cr _{0.27} Fe _{0.15} Ni _{0.15}	4	48	51	0	2	1	29.4	12.9

*FCC indexing is more likely to be a variation in the distorted BCC structure.

The three alloy samples were indexed for the known present phases from XRD using precession electron diffraction (PED) in TEM. The results confirm that the alloys were primarily BCC with some small amounts (<10%) of potential oxide structures within the film. In alloy #4 approximately 51% of the diffraction patterns in the small field of view are indexed to the FCC reference structure (See Supplementary

S10). When FCC was included in the indexing for #81 and #111, only 4% of points indexed to it. These locations were investigated and determined to be distorted BCC structures that were either inadequately described by the chosen distortion lattice parameters or had overlapping structures that introduced a reflection that skewed the result. The authors consider these indexed points to be indicative of variations in distortion and complexity of the microstructure and should be included in the BCC total. The relative difference in indexed points between #111, #81, and #4 indicates that FCC was an improved match from the distorted BCC reference specifically in #4. Overlap of the matrix BCC structure and the FCC content could explain the 51% content that is not in agreement with the lab XRD findings. The indexing of the diffraction patterns also produced orientation maps that were used to determine the average grain size via hand selection in ImageJ. These results provide some insight into the similarity of the structures between positions on the wafer. #111 and #81 were observed to have larger grains than #4. Grain dilation was performed on the orientation maps, and the results are provided as well for comparison. They skew low due to the noise in both samples, but the trend of #4 having a small grain size is in agreement with the manual measurements. Besides the presence of the FCC phase, oxides were found in 5% or less of the area in all three positions. Oxide content may be negligible.

Thermodynamics - CALPHAD

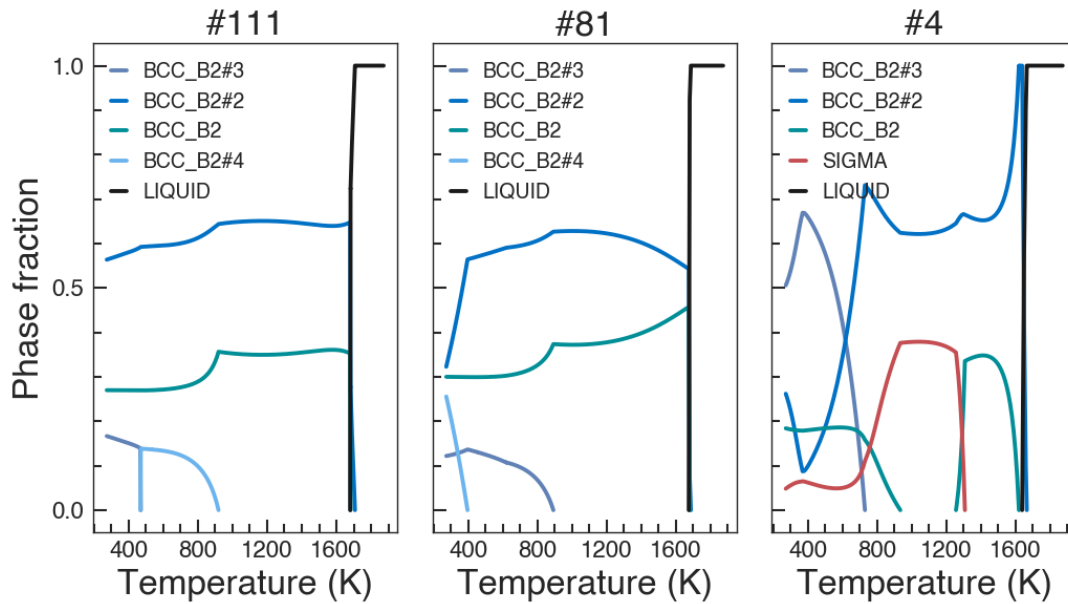


Fig. S8. One axis equilibrium phase diagram with phase fraction vs temperature of all three down selected samples generated using the TCHEAv3.2 database of Thermocalc.

Fig. S8 shows a Thermocalc generated one axis diagram of #111, #81 and #4 created to check the thermodynamically stable phases expected at 400 °C (673 K) - annealing temperature of the thin film library. The BCC_B2, BCC_B2#2, BCC_B2#3, and BCC_B32#4 phases have the same ordered structure (Ni-Al type) but could have different compositions. The TC-Python package provided by the Thermocalc 2021a version was used.

X-ray Diffraction

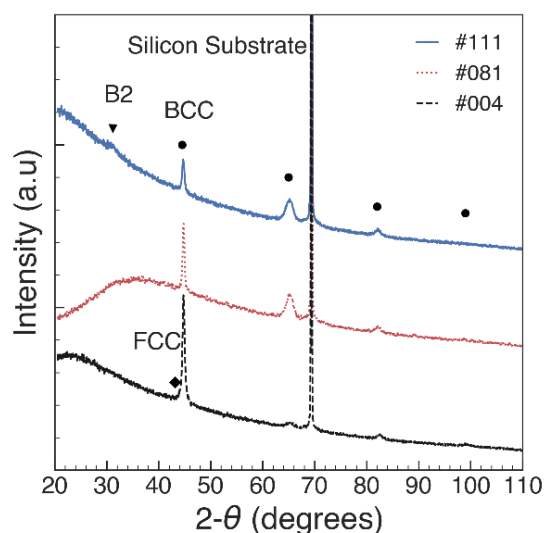


Fig. S9. XRD of the unexposed regions of #4, #81 and #111 with wider range from HTp XRD.

Alloy #81 was observed to have a small B2 peak (<5% of max intensity peak), while alloy #111 had intensity near the B2 position but it was not distinguishable from background in the initial scan. Both were selected as likely single-phase alloys with good corrosion resistance, and alloy 4 was selected for comparison because it exhibited the worst performance in passivation within the designated single-phase BCC* region. A wider 2-theta scan was performed on the three positions of interest to confirm their structures and are presented in the supplementary material, **Fig. S9**. The wider 2-theta scan confirmed that alloy 111 exhibits a B2 peak and no other peaks besides at the expected BCC positions. Alloy 4 had higher intensity with an additional BCC reflection compared to the other two alloys, though otherwise did not reveal any additional FCC peaks. The peak shape and intensity on the left shoulder suggest some FCC that is not detectable through XRD alone. Low certainty transition zones designated as “Maybe RSS” were observed in each wafer between the high confidence of single-phase structures, and the intermetallic containing regions. Alloy 4 was adjacent to a clear transition zone, and thus it was suspected that there was remaining FCC. Further investigation via TEM to confirm secondary phases and incorporation of Rietveld analysis of the XRD data in down selection may be useful to detecting small but nonetheless present phases via high-throughput XRD. Further attention was given to what type of intermetallic phases and crystal structure were present in all the spots.

Long term passive film performance and XPS analysis for oxide compositions

Echem: Potentiostatic electrochemical impedance spectroscopy (EIS) was performed on the exposure modified native oxide covered CCA surface after exposure at the open circuit potential (OCP) for 1800 s, with a 20 mV (RMS) amplitude AC signal from 100 kHz to 10 mHz¹. The remaining native oxide was then cathodically reduced at -1 V for 120 s. An OCP was observed for 5 s to perform a linear sweep voltammetry (LSV) from -0.2 V vs. OCP to 1 V vs. SHE at a scan rate of 20 mV/s. For XPS, the air formed oxide film was cathodically reduced following the same protocol mentioned above and then the solution formed passive film was grown following a potentiostatic polarization at 0.6 V vs SHE for 10 ks

¹ This entire sequence can be completed in less than an hour and the EIS frequency sweep in a few hundred seconds.

To mitigate potential bias from the initial LSV experiments, which can significantly alter the alloy composition through dissolution or delamination, the single step passivation experiments were performed at adjacent spots of the exposure. The range of passivation was determined from the LSV and used to define a suitable passivation potential of 0.6 V for passivation and EIS after 10 ks to assess healing after the native oxide is reduced and long term passivation behavior for down-selected alloys three alloys (two excellent and one inferior).

XPS: The energy and time per step were 0.05 eV and 50 ms, respectively. The instrument was calibrated with an Au standard to the 4f_{7/2} core level at 84.00 eV binding energy. Relative atomic sensitivity factors as provided by PHI were used to normalize elemental contributions. All peaks were shifted using C 1s = 284.8 eV and deconvoluted with Shirley background subtractions, Doniach-Sunjic convoluted with Gaussian peaks for metallic features, and Voigt functions for oxidized features using KOLXPD™ software package. Metal and oxidized peaks were identified from reference spectra of Al [4] and Cr, Fe, Co, Ni first-row transition [5] elements. A constant binding energy shift for each compound in Fe and Co 2p_{1/2} spectra relative to their reference 2p_{3/2} spectra was assumed. It is unclear if the small Fe, Ni, and Co signals are present as solute captured cations [6] in Al or Cr oxides, form phase separated undetected spinels or simple stoichiometric oxides such as NiO or Fe₂O₃, or actively dissolve during growth of the Al-Cr passive film when grown for 10 ks. These results differ from what would be expected of the air formed oxide.[7,8]

EXAFS analysis

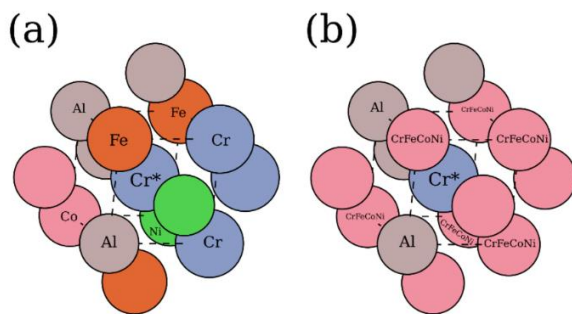


Figure S10. (Repeated Figure 2 of the manuscript) A Schematic diagram of Cr local environment used to parameterize the EXAFS models. Dashed lines indicate the BCC unit cell with the absorbing atom Cr* at the body centered site. **(a)** Without simplifying assumptions, the atomic cluster used for EXAFS analysis must contain all five species in the first (annotated with chemical symbols) and second neighbor shells. **(b)** A pseudo binary structural model with composite species for all transition metal scatterers $M = \{Cr, Fe, Co, Ni\}$.

EXAFS raw data were reduced using Larch[9] and Demeter software packages.[10] Quantitative analyses were performed on the Cr and Ni K-edges of samples #81 and #111, using FEFF6 to fit the data in r space. **Figure S110** shows the structural model used in this analysis. Fitting the unsimplified structural model in **Figure S10a** would be challenging because it is highly overparameterized relative to the limited information in the individual Cr/Ni EXAFS spectra; assuming negligible vacancies, each neighbor shell introduces four independent coordination number (CN) variables, five bond lengths, and five mean squared relative displacement parameters (MSRD or σ^2), for a total of 28 structural parameters. In addition to this high degree of overparameterization and the usual high degree of degeneracy between *e.g.*, MSRD and coordination numbers,[11] the transition metal elements in the film have very low Z contrast. The resulting similarity in the scattering signal from the transition metals introduces extreme degeneracies between the

corresponding structural parameters, especially for Cr, Fe, Co, and Ni scattering species.[12] To simplify quantitative analysis of the single-edge Cr/Ni EXAFS, we introduce the assumptions illustrated by **Figure S10b**, modeling the Cr, Fe, Co, and Ni scatterers as a single composite species, M. This reduces the degree of overparameterization, but it limits our quantitative insight for each coordination environment to just the Cr-Al / Ni-Al versus Cr-M /Ni-M short range order behavior, respectively.[12]

The simplified model of **Figure S1S10b** shown in the manuscript has two independent CN parameters, four bond lengths, and four MSRD parameters. EXAFS analyses were performed on the two edges Cr, and Ni K-edges. In our analysis, we used the Cr scattering signal for the composite species, “M.” Since the amplitude reduction factor S_0^2 for Cr and Ni is not independently resolvable from the coordination numbers, the S_0^2 was determined *a priori* using reference materials for the Cr and Ni K-edges and fixed at 0.92 and 0.81 for the fitting, respectively. To further constrain the problem, in case of the Cr K-edge, we applied equality constraints on the MSRD parameters for the first (1NN) and second (2NN) neighbor shells, so that $\sigma_{\text{Cr-Cr1NN}}^2 = \sigma_{\text{Cr-Cr2NN}}^2$ and $\sigma_{\text{Cr-Al1NN}}^2 = \sigma_{\text{Cr-Al2NN}}^2$. The interatomic distance R , and coordination numbers for the first and second nearest neighbors (1NN and 2NN, respectively) were varied independently. The model was further simplified for the Ni K-edge, by placing a constraint on the 2NN neighbor shell to contain exclusively Ni-M pairs.

It is convenient to describe the coordination numbers derived from EXAFS analysis as the conditional probability of each species occupying the neighbor shells of the absorbing atom, which we can combine with we quantified the CSRO using the classic pairwise Warren Cowley (WC) parameters. [13,14] The WC parameter α_{ab}^r normalizes the conditional neighbor probabilities between pairs of species a and b in the r^{th} NN shell to average composition:

$$\alpha_{ab}^r = \alpha_{ba}^r = \begin{cases} 1 - \frac{P_r(b|a)}{P(b)} = 1 - \frac{P_r(a|b)}{P(a)} & a \neq b \\ \frac{P(b) - P_r(b|a)}{P(b) - 1} & a = b \end{cases}$$

$P_r(b|a)$ is the conditional probability of species B appearing in the neighborhood of species A as a fraction of sites in that r^{th} shell. $P(a)$ and $P(b)$ are the nominal compositions of species A and B , respectively, and δ_{ab} is an indicator function that takes the value 1 when a and b represent the same species and 0 otherwise. For the rest of this discussion, we drop the neighbor shell index r for notational simplicity. The WC CSRO parameter is a convenient tool for CSRO analysis because a value $\alpha_{ab} = 0$ indicates no statistical neighbor preference between species A and B , $\alpha_{ab} > 0$ indicates fewer $A - B$ neighbors than in a random configuration (clustered CSRO), and $\alpha_{ab} < 0$ indicates more $A - B$ neighbors (ordered CSRO) than random.

In binary solid solutions, the largest span of Warren Cowley (WC) parameter values is obtained for the equiatomic stoichiometry: $-1 \leq \alpha_{ab} \leq 1$. However, this result does not generalize to ternary and higher-order alloy systems where it is possible to have multiple dilute species. In this case, the smallest possible lower bound of the α_{ab} diverges to negative infinity when both species A and B approach the dilute limit.

$$\lim_{\substack{P(a) \rightarrow 0 \\ P(b) \rightarrow 0}} \alpha_{ab} = -\infty$$

In N -component solid solutions there are N^2 WC parameters, $N(N - 1)/2$ of which are linearly independent. [15] These constraints derive from the symmetry imposed by definition of conditional probability, which implies that $\alpha_{ab} = \alpha_{ba}$. The feasible values for these WC parameters depend on the

nominal compositions as before. de Fontaine[15] also identifies several more stringent mathematical bounds for the WC parameters in multicomponent solid solutions, namely the quadratic constraints identified by . However, these constraints couple across pairs of components so that the limits for a given WC parameter α_{ac} depends on the values of the other WC parameters (α_{ab} , α_{bc} , etc.). Because in the current work we are only able to quantify the WC parameter for the pseudo-binary model, we are not directly able to check these constraints. However, in a forthcoming work we analyze in detail the nature of this cross-coupling of WC parameters with the goal of better understanding SRO in multicomponent alloys and developing efficient and more straightforward application of these constraints in the nonlinear least squares model optimization commonly used in EXAFS analysis.

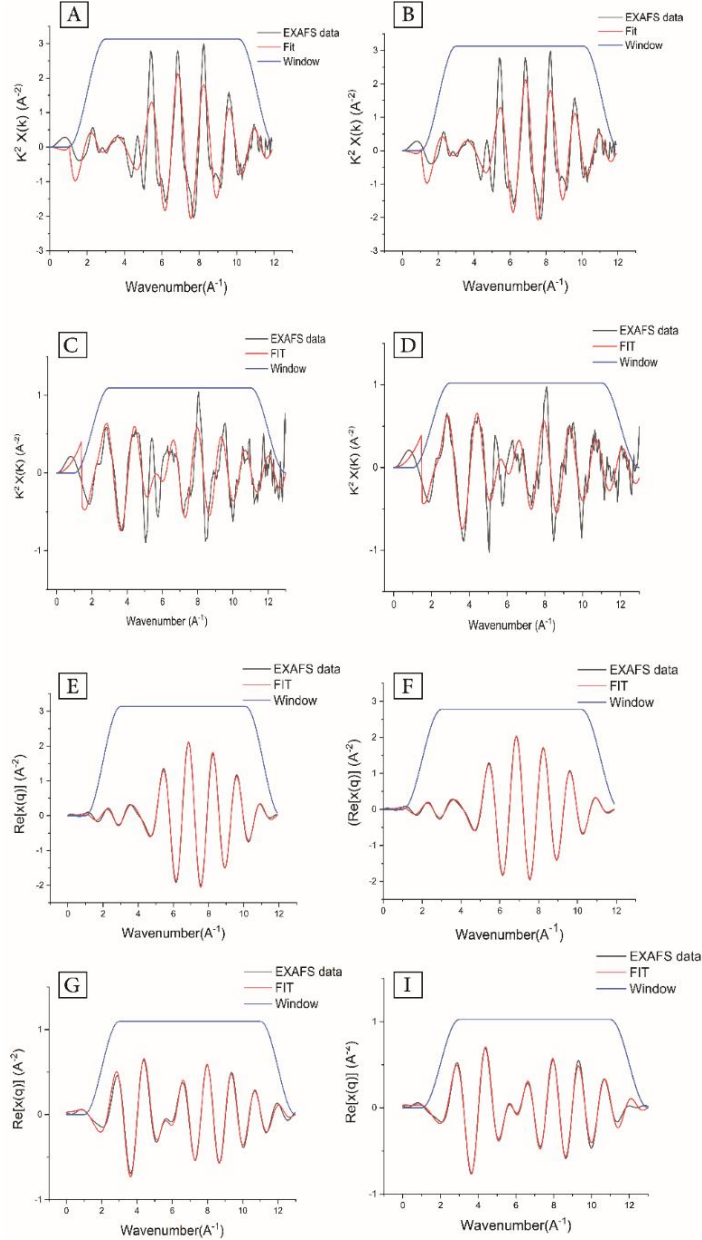


Fig. S11. Fourier filtered EXAFS spectra in k space of Cr K-edge of (A) #81 and (B) #111 and Ni K-edge of (C) #81, and (D) #111. Extracted EXAFS spectrum spectra of Cr K-edge of samples (E) #81 and (F) #111 and Ni edge of samples (G) #81 and (I) #111, transformed in q-space.

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