



Short communication

## Reversible poisoning of nickel/zirconia solid oxide fuel cell anodes by hydrogen chloride in coal gas

O.A. Marina<sup>a,\*</sup>, L.R. Pederson<sup>b</sup>, E.C. Thomsen<sup>a</sup>, C.A. Coyle<sup>a</sup>, K.J. Yoon<sup>a</sup><sup>a</sup> Pacific Northwest National Laboratory, Richland, WA, United States<sup>b</sup> North Dakota State University, Fargo, ND, United States

## ARTICLE INFO

## Article history:

Received 15 April 2010

Received in revised form 1 May 2010

Accepted 4 May 2010

Available online 7 May 2010

## Keywords:

Ni/YSZ anode

HCl

Chlorine adsorption

SOFC performance

Coal contaminants

## ABSTRACT

The performance of anode-supported solid oxide fuel cells (SOFC) was evaluated in synthetic coal gas containing HCl in the temperature range 650–850 °C. Exposure to up to 800 ppm HCl resulted in reversible poisoning of the Ni/zirconia anode by chlorine species adsorption, the magnitude of which decreased with increased temperature. Performance losses increased with the concentration of HCl to ~100 ppm, above which losses were insensitive to HCl concentration. Neither cell potential, nor current density had any effect on the extent of poisoning. No evidence was found for long-term degradation that can be attributed to HCl exposure. Similarly, no evidence of microstructural changes or formation of new solid phases as a result of HCl exposure was found. From thermodynamic calculations, solid nickel chloride phase formation was shown to be highly unlikely in coal gas containing HCl. The presence of HCl at even the highest anticipated concentrations in coal gas would minimally increase the volatility of nickel.

© 2010 Elsevier B.V. All rights reserved.

### 1. Introduction

Solid oxide fuel cells (SOFCs) can utilize a wide variety of fuels including coal-derived syngas, and coal-based SOFC-gas turbine hybrid systems are expected to achieve greater than 50% higher heating value (HHV) efficiency [1–4]. In the coal gasification process, coal is mixed with oxidant and/or steam to produce synthesis gas that consists primarily of CO, H<sub>2</sub>, CO<sub>2</sub>, H<sub>2</sub>O, CH<sub>4</sub>, and N<sub>2</sub>. Multiple minor and trace impurities that are present in coal may remain in the gasified coal even after cleanup, which could affect SOFC performance and lifetime [5]. Since various impurities may affect the cell performance in different ways, it is important to understand the interactions between the SOFC anode and each impurity to enable the long-term performance of an SOFC stack operated on coal gas to be predicted.

Chlorine is among the impurities found in coal that could have consequences for SOFC operation. Found in concentrations from 0.01 to 1% by weight principally in the form of sodium and potassium chlorides, chlorine is widely distributed in coals [6]. Nearly all of the chloride salts will be converted to HCl in coal-derived synthesis gas, with concentrations as high as 500 ppm reported [7]. Although aqueous scrubbing is expected to remove most HCl, as much as a third could still remain [7,8]. Through the use of solid sor-

bents such as CaO, HCl concentrations  $\lesssim$  ppm can be achieved [9,10].

Chlorine is a well-known poison of transition metal-catalyzed reactions, particularly those involving hydrogen and carbon monoxide [11–15]. For example, Richardson et al. have found that catalytic activity of nickel towards methane reforming, water gas shift reactions and chlorocarbon-steam reforming was effectively poisoned in the presence of HCl [13,14]. Attributed to the formation of surface chloride species, the poisoning effect was reversible: nickel activity was restored after exposure to chlorine-free steam [13,14]. Kiskinova and Goodman have found that pre-adsorbed Cl atoms on Ni(100) led to a reduction of the sticking coefficient, the adsorption bond strength, and the adsorption capacity of that surface for CO and H<sub>2</sub> [16]. Zhuang et al. reported similar results for Cl pre-adsorbed on the Ni(110) surface, and additionally found that Cl could displace pre-adsorbed CO [17]. Chlorine was found to adsorb on high symmetry fourfold or threefold hollow sites, even at saturated coverage, with little or no surface reconstruction [18–20].

The effects of HCl on SOFC performance has been addressed previously in several studies [7,21–29], with varied results. Veyo found no impact of 1 ppm HCl in synthetic coal gas on the performance of a tubular SOFC operating at 1000 °C, a temperature considerably higher than that currently being considered for planar systems [21]. Aravind et al. found no changes in the performance of an electrolyte-supported planar SOFC upon short-term (~2 h) exposure to 9 ppm HCl at 850 °C, and concluded that the anode remained electrocatalytically active for hydrogen oxidation [22]. Similarly, Buchinger et al. observed no effect of 5 and 47 ppm HCl in dry

\* Corresponding author. Tel.: +1 509 375 2337; fax: +1 509 375 2186.  
E-mail address: [olga.marina@pnl.gov](mailto:olga.marina@pnl.gov) (O.A. Marina).

hydrogen on the performance of an electrolyte-supported micro-tubular SOFC in ~20 h tests at 850 and 900 °C [24]. An almost immediate but reversible performance loss of up to ~50 percent was observed by Tremblay et al. for electrolyte-supported cells exposed to 20 and 160 ppm HCl in synthetic coal gas at 800 and 900 °C, but the performance stabilized within 100 h [7]. Increases in electrodic resistance were principally observed and attributed to adsorption of Cl on electrochemically active reaction sites, while a minor increase in ohmic losses was attributed to degradation of the current collector that was unrelated to anodic processes [7]. Bao et al. studied the response of anode-supported cells at 750 and 800 °C to synthetic coal gas with 40 ppm HCl, and found no change in performance for periods up to 120 h [23]. Minor performance losses resulted from exposure of anode-supported cells to 40 ppm CH<sub>3</sub>Cl at 850 °C, however [23]. Xu et al. reported a steady and permanent loss in performance of ~3% over 400 h at 800 and 850 °C for anode-supported cells exposed to 100 ppm HCl in synthesis gas [25]. Minor surface reconstruction of the nickel anode was observed, as was evidence for adsorption of chlorine onto nickel surfaces [25]. Haga et al. reported a steady degradation of electrolyte-supported cells during 150 h exposures to 5–1000 ppm Cl<sub>2</sub> in 3%-humidified hydrogen at 800 °C [26,27]. The degradation rate increased with increasing chlorine concentration from 3%/1000 h for 5 ppm Cl<sub>2</sub> to 94%/1000 h for 1000 ppm Cl<sub>2</sub>, accompanied by significant microstructural changes in the nickel anode that were attributed to solid NiCl<sub>2</sub> formation and sublimation. Suggested poisoning mechanisms included both reversible chlorine adsorption on Ni surfaces and irreversible nickel redistribution via NiCl<sub>2</sub> formation [26,27]. Bao et al. reported that the presence of HCl in fuel gases could be beneficial to fuel cell performance, by helping to mitigate the effects of other coal gas impurities such as As and P [28]. We have also reported that HCl exposure can improve fuel cell performance by lowering ohmic losses in 8 mol% yttria-stabilized zirconia (YSZ) [29]. These effects were attributed to volatilization as chlorides of some of the Mn that had diffused from the cathode through the electrolyte to the anode side during processing. No such effects were found for cells with non-Mn-containing cathodes, consistent with this interpretation [29].

The present study was undertaken because of a general lack of agreement in previous investigations with regard to whether Cl in coal gas does indeed lower the performance of an SOFC, whether those performance changes are reversible, or whether Cl exposure results in microstructural changes in the Ni-based anode. In the present work, the Ni/YSZ anode-supported SOFCs were tested for extended periods in synthetic coal gas containing 5–800 ppm HCl in the temperature range 650–850 °C. Temperatures lower than those considered previously were included to emphasize any effects of surface adsorption. The effect of HCl on the cell performance was investigated using electrochemical dc and ac measurements. Post-test analyses using electron microscopy and surface analytical probes were performed to establish the extent of Cl uptake by Ni and whether changes in anode morphology had occurred.

## 2. Experimental

Cell tests were conducted using nickel/zirconia anode-supported cells. Button cells with an active area of 2 cm<sup>2</sup> were fabricated as described previously [30]. The anode support was approximately 900 μm thick and 30 vol.% porous, and was comprised of a Ni/YSZ bulk layer with a 40/60 vol.% ratio. The anode active layer was 5 μm thick and composed of 50/50 vol.% Ni/YSZ. The 8 mol% YSZ electrolyte was 9 μm thick. The anode-electrolyte structure was pre-sintered at 1375 °C, and a 2 μm thick samaria-doped ceria (SDC) barrier layer was applied by screen printing and sintered at 1200 °C. A 30–50 μm thick (La<sub>0.8</sub>Sr<sub>0.2</sub>)<sub>0.98</sub>MnO<sub>3</sub> (LSM-

20) cathode was screen-printed and sintered at 1100 °C for 2 h. The anode current collector, comprised of Ni mesh, was embedded in NiO paste and co-fired with the ceria. The cathode current collector was Ag foil grid impregnated with Ag paste and sintered in situ during seal curing. Cells were sealed to alumina test fixtures with a barium aluminosilicate glass by heating to 850 °C in air. The anode was reduced in situ at 850 °C by moist hydrogen saturated with water at room temperature.

Cell tests were performed in the temperature range 650–850 °C. The synthetic coal gas was created by equilibrating 55 parts by volume hydrogen with 45 parts by volume carbon dioxide, and used as a fuel gas. This mixture was equilibrated over a catalyst bed consisting of Ni/YSZ at 700 °C prior to introduction of the contaminant, yielding a nominal composition of H<sub>2</sub>/CO/CO<sub>2</sub>/H<sub>2</sub>O = 30%/23%/21%/26%. Cells were pre-conditioned in synthetic coal gas at 0.7 V for 20–100 h to obtain a stable baseline prior to exposure to HCl. Cells were further conditioned in synthetic coal gas containing 100 ppm HCl for an additional 100 h to stabilize ohmic contributions associated with phenomena described elsewhere [29]. The cathode was supplied with essentially pure oxygen from a pressure swing adsorption unit. This approach results in a small and constant cathodic polarization contribution. Hydrogen chloride was supplied from cylinder using calibrated electronic flow controllers and added to the synthetic coal gas through a separate gas channel directly to the anode, thereby by-passing the Ni catalyst. Arbin Instruments multichannel controllers and a Solartron Model 1255/1470 Multistat test system were used for electrochemical tests. The latter, in addition to a Solartron Model 1260/1287 instrument, was used to obtain electrochemical impedance spectra. During such HCl exposure tests, impedance data were obtained at random time intervals at the same bias current for all of the cells. Following termination of electrochemical tests, individual cells were analyzed using scanning electron microscopy (SEM) with energy dispersive spectroscopy (EDS) and Auger electron spectroscopy (AES).

## 3. Results

A modest but rapid decrease in cell performance was characteristically observed upon introduction of various concentrations of HCl to synthetic coal gas, with rapid recovery observed when HCl exposure ceased. Typical results are shown in Fig. 1, which corresponds to a cell operating at a constant potential of 0.8 V in coal gas with 50 ppm HCl at 700 °C. Within a few hours of HCl exposure, the output of this cell decreased by ~3%, and essentially completely

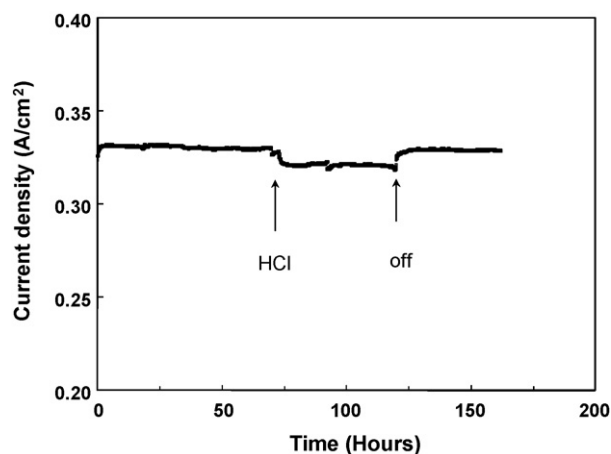
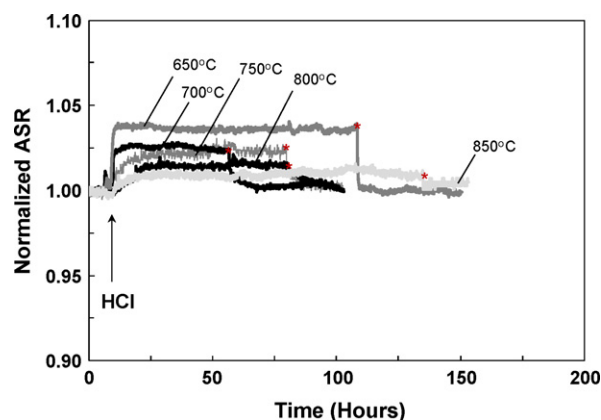


Fig. 1. Current density generated by the Ni/YSZ anode-supported cell at a cell potential of 0.8 V in the presence of 50 ppm HCl in coal gas at 700 °C.

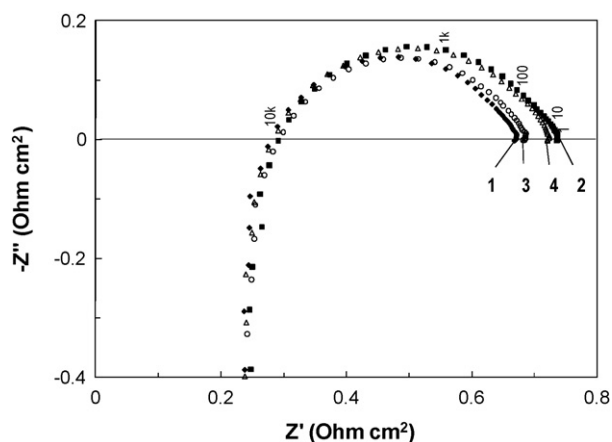


**Fig. 2.** Normalized area-specific resistance (ASR) of Ni/YSZ anode-supported cells in the presence of 50 ppm HCl at different temperatures (calculated as ASR in coal gas with HCl over ASR in coal gas without HCl). Cells were operated at a constant potential of 0.8 V. Asterisks mark the moment when HCl was shut off for each cell.

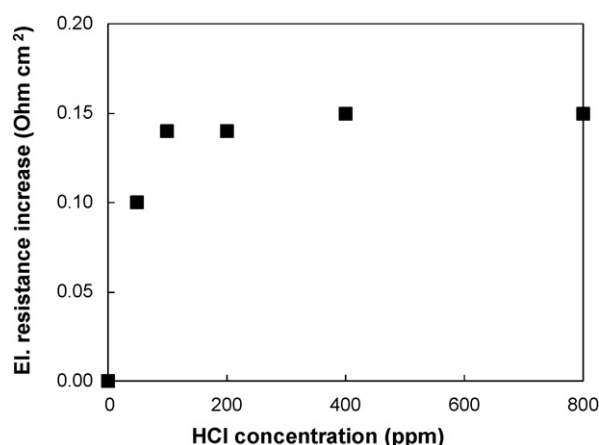
recovered within a few hours when exposure ceased. No long-term loss in performance due to HCl exposure could be discerned.

Similar rapid and reversible responses to HCl exposure were observed at other temperatures as well. Fig. 2 shows changes in the normalized area-specific resistances (ASR) due to exposure of cells to 50 ppm HCl in synthetic coal gas from 650 to 850 °C. Normalized ASR is defined as ASR in coal gas with HCl divided by ASR in clean coal gas at a given temperature and current density. Though cathodic and electrolyte losses contribute to the magnitude of the ASR, changes are attributed solely to HCl exposure. At each temperature, the normalized ASR increased quickly upon exposure to HCl, and recovered quickly and fully when exposure ended. The magnitude of performance change was found to be greatest at 650 °C, and least at 850 °C. No differences in rates of recovery were apparent in this temperature range.

Electrochemical impedance measurements revealed that this reversible performance loss was electrodic in nature. Fig. 3 compares spectra obtained at 700 °C at constant current density in clean coal gas and in coal gas containing 200 ppm HCl. The width of the dispersion arc, a measure of the sum of cathodic and anodic losses, increased modestly upon HCl exposure, and recovered effectively in clean coal gas. It is reasonable to assume that changes are due only to anodic processes, given that conditions did not change at the



**Fig. 3.** Nyquist plots of impedance spectra of anode-supported cells obtained initially in clean coal gas (1), after 50 h of exposure to 200 ppm HCl (2), immediately after HCl was removed from coal gas (3), and again after repeated 75 h exposure to 200 ppm HCl (4) at 700 °C. Bias current is 0.25 A cm<sup>-2</sup>. Frequencies are marked above the spectra.



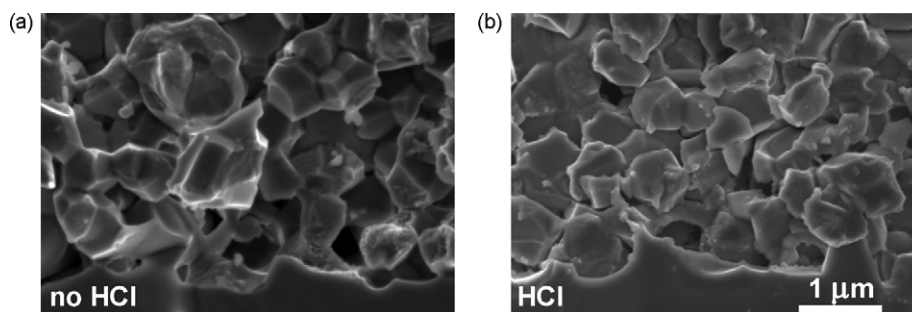
**Fig. 4.** Change in electrodic resistance of Ni/YSZ anode-supported cells due to the exposure to various concentrations of HCl in synthetic coal gas at 700 °C. The magnitude of resistance change for a given HCl concentration decreased with increased temperature, though showed similar trends versus HCl concentration.

cathode. The electrolyte resistance, determined from the high frequency intercept with the real impedance axis, remained constant. It is noted that these cells were conditioned in 100 ppm HCl prior to these measurements to stabilize the electrolyte resistance. Our prior work has shown that initial exposure to HCl actually results in lowered electrolyte resistance, due to volatilization of Mn that had diffused through the electrolyte to the anode side during processing [29].

Performance losses were insensitive to the concentration of HCl in coal gas, for concentrations greater than ~100 ppm, as shown in Fig. 4 for cells exposed to 0–800 ppm HCl in coal gas at 700 °C. Below 100 ppm HCl, cell resistance changes increased approximately linearly with HCl concentration. Similar trends in cell resistance versus HCl concentrations were observed at other temperatures. However, the magnitude of the HCl-induced changes was suppressed as temperature was increased. The effect of cell potential, or cell current density, on cell degradation in the presence of HCl was evaluated as well. No clearly distinguishable change in the degradation rate due to the HCl presence was observed in wide current density range from 0.1 to 1 A cm<sup>-2</sup>.

Post-mortem characterization of the several Ni/YSZ anodes tested in HCl was performed using field emission SEM/EDS. For comparison, similar analysis was performed on Ni/YSZ anodes tested in coal gas only. Typical microstructures for cells tested in synthetic coal gas with and without HCl are compared in Fig. 5. No changes in microstructure due to HCl exposure were apparent following 800 h operation in coal gas with or without HCl present. Edges of nickel grains remained identically sharp. There was no etching or pitting that could be associated with reactions with chlorine. No indication of the presence of any chlorine-containing nickel compounds was found.

Additionally, AES, which is sensitive to nominally the outer 10 nm of a sample surface, was employed to evaluate whether evidence of chlorine-containing reaction products or a surface adsorption layer was present. Auger spectra were collected from both single Ni particles and from the Ni/YSZ area inside the Ni/YSZ bulk anode. Chlorine adsorption was detected, but only in relatively small amounts (1.5–2% relative to nickel). There was no evidence of Cl enrichment on Ni particles or any chlorine-containing solid phases. It is noted that these samples were cooled in hydrogen gas without HCl, and were additionally exposed to air for several days prior to AES analysis, which may have resulted in partial chlorine loss from an adsorption layer. As such, these concentrations should be considered to be a lower bound.



**Fig. 5.** SEM images of the Ni/YSZ active anode near the YSZ electrolyte tested for 800 h in (a) clean coal gas and (b) coal gas with 50 ppm HCl. No microstructural changes are apparent.

#### 4. Discussion

The presence of HCl in coal gas was found to result in minor losses in SOFC performance, and those losses were largely reversible. Performance losses are attributed to the effects of HCl adsorption, probably dissociative, onto nickel surfaces at the active anode/electrolyte interface, which lowered the activity of the nickel electrocatalyst. Long-term degradation attributable to HCl in coal gas could not be discerned, and no changes in the composition or microstructure of the anode were apparent. From thermodynamic calculations, solid nickel chloride phase formation is considered to be highly unlikely in coal gas. Further, the presence of HCl at even the highest anticipated concentrations is not expected to significantly increase the volatility of nickel.

Surface adsorption of chlorine onto nickel electrocatalyst surfaces is concluded to be the principal cause of losses in SOFC performance. Observations supporting that conclusion include the following: (1) losses were reversible, with cells recovering their initial activity within a few hours when HCl exposure ceased; (2) performance losses were essentially independent of HCl concentration for concentrations  $\geq 100$  ppm, implying a saturation coverage; (3) the magnitude of performance losses for a given HCl concentration in coal gas decreased with increased temperature; (4) HCl-induced changes in performance were electrodic in nature, implying temporary loss of electrocatalytic activity; and (5) no evidence of changes in microstructure or the formation of new chloride-containing solid phases was found. Very similar reversible Ni anode poisoning was observed for the YSZ-electrolyte-supported cells [29].

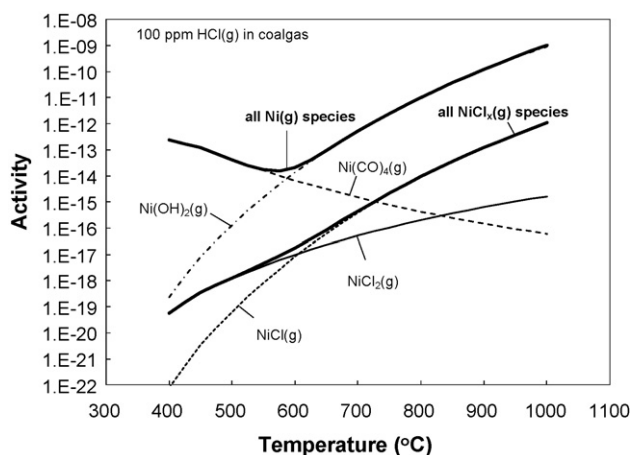
Tremblay et al. similarly observed rapid, reversible degradation of Ni-based anodes in the electrolyte-supported cells due to HCl exposure, and attributed these observations to surface adsorption of chlorine-containing species [7]. Chlorine is a well-known poison of transition metal-catalyzed reactions, which occurs through the adsorption of surface-active chlorine species [11–15]. The effects of chlorine adsorption on the activity of nickel steam reforming catalysts have been shown to be reversed by exposure to chlorine-free steam [13,14], indicating that the strength of the adsorptive bond is not excessively large. Previous studies have revealed that pre-adsorption of Cl onto Ni surfaces lowered the sticking coefficient, the adsorption bond strength, and the adsorption capacity of those surfaces for CO and H<sub>2</sub> [16,17], which helps to explain losses in catalytic activity due to Cl adsorption. Consistent with the finding of high reversibility for chlorine poisoning of nickel catalysts, the adsorption of chlorine was not accompanied by surface reconstruction [18–20].

The fact that anode poisoning due to HCl exposure has not been observed in several previous studies may be attributed to a combination of high SOFC operating temperature and low HCl concentrations, both of which would lower the extent of surface adsorption. For example, Veyo found no effect of 1 ppm HCl at

1000 °C [21], Aravind et al. reported no effect of short-term (~2 h) exposure of 9 ppm HCl at 850 °C [22], and Buchinger et al. determined that exposure to 5 and 47 ppm HCl at 850 °C caused no loss in performance [24]. On the other hand, Bao et al. found no poisoning for HCl concentrations of 40 ppm at 750 and 800 °C for up to 120 h [23], conditions that led to discernable though small loss of performance in the present study.

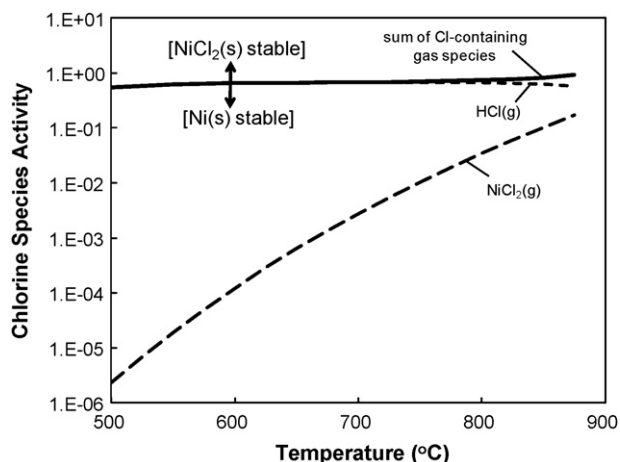
No long-term degradation was found in the present work for cells that had been pre-conditioned in synthetic coal gas containing HCl. The principal reason for pre-conditioning was to stabilize ohmic contributions to overall cell resistance due to phenomena described earlier [29]. In that study, it was found that Mn concentrations in grain boundaries at the anode/electrolyte interface of anode-supported cells were lowered by HCl exposure, resulting in a reduction in electrolyte ohmic resistance over periods of ~100 h. Cells constructed with other than Mn-based cathodes did not show this effect [29]. Minor increases in ohmic losses have been found due to HCl exposure by Tremblay et al. over a period of ~100 h, though these effects were attributed to electrical contact instability [7]. Long-term instability due to HCl exposure was reported as a result of at least two studies. Xu et al. found steady and permanent degradation of ~3% over 400 h at 800 and 850 °C in 100 ppm HCl in coal gas, accompanied by surface reconstruction of the nickel anode [25]. Haga et al. reported extensive and permanent degradation as a result of exposure of 5–1000 ppm Cl<sub>2</sub> in humidified hydrogen, which was attributed to solid NiCl<sub>2</sub> formation and sublimation [26,27].

From thermodynamic considerations, the presence of expected concentrations of HCl in coal gas should neither significantly increase volatilization of nickel, nor lead to the formation of NiCl<sub>2</sub>



**Fig. 6.** Expected activities of gaseous nickel-containing species in synthetic coal gas with 100 ppm HCl versus temperature, calculated using FactSage v. 6 [31]. The presence of HCl is expected to negligibly enhance the volatility of nickel.





**Fig. 7.** Expected activities of gaseous nickel-containing species in synthetic coal gas needed to form stable  $\text{NiCl}_2(\text{s})$ , calculated using FactSage v.6 [31].  $\text{NiCl}_2(\text{s})$  is stable for conditions above the solid line, while Ni metal is stable for conditions below that line. Formation of  $\text{NiCl}_2(\text{s})$  in coal gas is highly unlikely.

solid phases. Activities of nickel vapor species at equilibrium in coal gas containing 100 ppm HCl are given in Fig. 6 versus temperature, calculated using the commercial software package FactSage v. 6 [31]. The sum of activities for  $\text{Ni}(\text{OH})_2(\text{g})$  and  $\text{Ni}(\text{CO})_4(\text{g})$ , which are unrelated to the HCl content in coal gas, are predicted to exceed the sum of activities for all  $\text{NiCl}_x(\text{g})$  species by approximately three orders of magnitude. As such, structural rearrangements due to chlorine-enhanced vapor transport of Ni at the anode/electrolyte interface are not expected. Consistent with these calculations, the adsorption of chlorine on nickel catalyst surfaces did not lead to surface reconstruction [18–20]. Further, as is shown in Fig. 7, it is not practically possible to form solid  $\text{NiCl}_2$  in coal gas containing realistic amounts of HCl. While HCl concentrations in coal gas of as high as 500 ppm may be possible [7], concentrations more than three orders of magnitude higher are needed to form solid  $\text{NiCl}_2$ .

## 5. Summary

Modest and reversible performance losses in SOFC performance were found to occur as a result of exposure to HCl in synthetic coal gas. These performance losses are attributed to the effects of adsorption of Cl species onto nickel surfaces at the active anode/electrolyte interface, consistent with conclusions of previous studies of nickel steam reforming catalyst poisoning by HCl. No evidence was found for long-term degradation that can be attributed to HCl exposure. Similarly, no evidence of microstructural changes or formation of new solid phases as a result of HCl exposure was found. Surface adsorption-related performance losses decreased with increased temperature, increased with the concentration of HCl to  $\sim 100$  ppm, and were essentially independent of HCl concentration above that value. From thermodynamic calculations, solid nickel chloride phase formation is considered to be highly unlikely in coal gas. Further, the presence of HCl at even the highest anticipated concentrations is not expected to significantly increase the volatility of nickel.

## Acknowledgements

We would like to acknowledge technical assistance of C.N. Cramer and J. Bonnet. SEM and FESEM analysis was performed by Dr. D. Edwards and B. Arey. Auger analyses were performed by A.S. Lea. Support for this work is provided by the U.S. Department of Energy, Office of Fossil Energy, National Energy Technology Laboratory through the SECA Coal-Based Systems Core Research Program. Pacific Northwest National Laboratory is operated for the US Department of Energy by Battelle under Contract ACO6-76RLO 1830.

## References

- [1] M.C. Williams, J.P. Strakey, W.A. Surdoval, J. Power Sources 143 (2005) 191–196.
- [2] M.C. Williams, J.P. Strakey, W.A. Surdoval, L.C. Wilson, Solid State Ionics 177 (2006) 2039–2044.
- [3] N.Q. Minh, ECS Trans. 7 (2007) 45–50.
- [4] T. Kivisaari, P. Bjornbom, C. Sylwan, B. Jacquinet, D. Jansen, A. de Groot, Chem. Eng. J. 100 (2004) 167–180.
- [5] J.P. Trembly, R.S. Gemmen, D.J. Bayless, J. Power Sources 163 (2007) 986–996.
- [6] Y.E. Yudovich, M.P. Ketris, Int. J. Coal Geol. 67 (2006) 127–144.
- [7] J.P. Trembly, R.S. Gemmen, D.J. Bayless, J. Power Sources 169 (2007) 347–354.
- [8] J. Ratafia-Brown, L. Manfredo, J. Hoffman, M. Ramezan, Major Environmental Aspects of Gasification-Based Power Generation Technologies, U.S. DOE NETL, 2002, pp. 39–59.
- [9] C.S. Chyang, Y.L. Han, Z.C. Zhong, Energy Fuels 23 (2009) 3948–3953.
- [10] B.L. Dou, W.G. Pan, J.X. Ren, B.B. Chen, J.H. Hwang, T.U. Yu, Energy Fuels 21 (2007) 1019–1023.
- [11] D.W. Goodman, Ann. Rev. Phys. Chem. 37 (1986) 425–457.
- [12] D.W. Goodman, J. Phys. Chem. 100 (1996) 13090–13102.
- [13] J.T. Richardson, J.D. Ortego, N. Couste, M.V. Twigg, Catal. Lett. 41 (1996) 17–20.
- [14] N. Couste, J.D. Ortego, J.T. Richardson, M.V. Twigg, Appl. Catal. B: Environ. 19 (1998) 175–187.
- [15] T.E. McMinn, F.C. Moates, J.T. Richardson, Appl. Catal. B: Environ. 31 (2001) 93–105.
- [16] M. Kiskinova, D.W. Goodman, Surf. Sci. 108 (1981) 64–76.
- [17] S.X. Zhuang, J.X. Wu, X.M. Liu, J. Tu, M.R. Ji, K. Wandelt, Surf. Sci. 331 (1995) 42–46.
- [18] T. Yokoyama, S. Terada, Y. Okamoto, M. Sakano, T. Ohta, Y. Kitajima, M. Tischer, K. Baberschke, Surf. Sci. 374 (1997) 243–250.
- [19] J. Zhang, Z.Y. Diao, Z.X. Wang, Chem. Res. Chinese Univ. 22 (2006) 488–492.
- [20] K. Asakura, H. Ishii, S. Konishi, Y. Kitajima, T. Ohta, H. Kuroda, Phys. B 208/209 (1995) 465–466.
- [21] S.E. Veyo, Evaluation of fuel impurity effects on solid oxide fuel cell performance, Final Technical Report, 1998 (DOE Contract No. DE-AC21-89MC26355-02).
- [22] P.V. Aravind, J.P. Ouweltjes, N. Woudstra, G. Rietveld, Electrochem. Solid State Lett. 11 (2008) B24–B28.
- [23] J. Bao, G.N. Krishnan, P. Jayaweera, J. Perez-Mariano, A. Sanjurjo, J. Power Sources 193 (2009) 607–616.
- [24] G. Buchinger, P. Hinterreiter, T. Raab, S. Griesser, R. Claassen, D.P. Claassen, W. Sitte, D. Meissner, J. Fuel Cell Sci. Technol. 3 (2006) 280–283.
- [25] C. Xu, M. Gong, J.W. Zhang, X. Liu, H. Finklea, J. Power Sources 195 (2010) 2149–2158.
- [26] K. Haga, Y. Shiratori, K. Ito, K. Sasaki, J. Electrochem. Soc. 155 (2008) B1233–B1239.
- [27] K. Haga, S. Adachi, Y. Shiratori, K. Itoh, K. Sasaki, Solid State Ionics 179 (2008) 1427–1431.
- [28] J.E. Bao, G.N. Krishnan, P. Jayaweera, A. Sanjurjo, J. Electrochem. Soc. 157 (2010) B415–B424.
- [29] O.A. Marina, L.R. Pederson, E.C. Thomsen, D.J. Edwards, C.A. Coyle, C.N. Cramer, Electrochem. Solid State Lett. 13 (2010) B63–B67.
- [30] C.A. Coyle, O.A. Marina, E.C. Thomsen, D.J. Edwards, C.N. Cramer, G.W. Coffey, L.R. Pederson, J. Power Sources 193 (2009) 730–738.
- [31] C.W. Bale, A.D. Pelton, W.T. Thompson, G. Eriksson, K. Hack, P. Chartrand, S. Deckerov, J. Menancon, S. Petersen, FactSage 6 ed., Thermfact and GTT-Technologies, 2007.