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### SOLID OXIDE FUEL CELL SYSTEM CHROMIUM POISONING PREVENTION MATERIALS

#### Abstract

A solid oxide fuel cell (SOFC) system includes a SOFC stack, a component located upstream from the SOFC stack and downstream from a heat exchanger, the component including a bulk portion; and a surface portion directly adjacent the bulk portion and having a combination of a sulfur getter material and a chromium getter material, the sulfur and chromium getter materials having different chemical compositions, the chromium getter being an absorber of hexavalent gaseous chromium and the sulfur getter being an absorber of sulfur-containing gaseous species.

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## Background/Summary

CROSS-REFERENCE TO RELATED APPLICATIONS [0001] This application is a continuation-in-part of U.S. application Ser. No. 18/487,636 filed Oct. 16, 2023, now pending, the disclosure of which is hereby incorporated in its entirety by reference herein.

### TECHNICAL FIELD

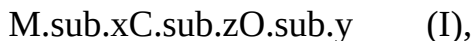
[0002] The present disclosure relates to electrochemical systems such as solid oxide fuel cell (SOFC) and electrolyzer systems, prevention of chromium and sulfur contamination and/or poisoning of the systems, especially minimizing release of previously bound hexavalent chromium, and methods of producing and using the same.

### BACKGROUND

[0003] High temperature electrochemical cells such as SOFC, like most fuel cell technologies, are at the forefront of power generation technology as they benefit the public and the planet by minimizing emissions such as NO<sub>x</sub>. Compared to proton exchange membrane fuel cell (PEMFC) that may be applicable for automotive applications, SOFCs are typically intended for stationary applications. SOFCs typically feature a relatively high combined heat and power efficiency, long-term stability, fuel flexibility, and low emissions. But SOFC devices run at relatively high operating temperatures, generating harsh operating conditions which have been a challenge from materials perspective. The harsh conditions also generate a need to prevent formation of any undesirable gaseous species in the system.

### SUMMARY

[0004] In one or more embodiments, solid oxide fuel cell (SOFC) system is disclosed. The system includes a SOFC stack and a component located upstream from the SOFC stack and downstream from a heat exchanger. The component may include a bulk portion and a surface portion adjacent the bulk portion and having a combination of a sulfur getter material and a chromium getter material, the sulfur and chromium getter materials having different chemical compositions, the chromium getter being an absorber of hexavalent gaseous chromium and the sulfur getter being an absorber of sulfur-containing gaseous species. The chromium getter material may not be a sulfur absorber. The sulfur getter material may be a sulfur and chromium absorber. The sulfur getter material may have a lower affinity to chromium than sulfur. Presence of the sulfur getter material within the combination may render the chromium getter material an irreversible chromium absorber. The sulfur getter material may include one or more than one composition having formula (I):



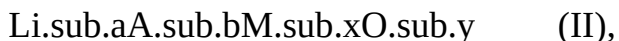
where M is an alkaline earth metal or alkali metal,

x is any number between 1 and 3,

y is any number between 1 and 4,

z is any number between 0 and 1.

[0005] The sulfur getter material may include one or more than one composition having formula (II):



where

A is a transition metal,

M is a metalloid or reactive non-metal,

a is any number between 1 and 4,

b is any number between 0 and 2,

x is any number between 0.1 and 3,

y is any number between 1 and 6.

[0006] The sulfur getter material may include  $\text{CaO}$ ,  $\text{MgO}$ ,  $\text{CaCO}_3$ ,  $\text{MgCO}_3$ ,  $\text{CaCrO}_4$ ,  $\text{MgCrO}_4$ ,  $\text{MgCr}_2\text{O}_4$ , or their combination, and the chromium getter material includes  $\text{BaO}$ ,  $\text{SrO}$ ,  $\text{BaCO}_3$ ,  $\text{SrCO}_3$ ,  $\text{BaCrO}_4$ ,  $\text{SrCrO}_4$ , or their combination.

[0007] In another embodiment, a SOFC component is disclosed. The component may include a bulk portion and a surface portion having a combination of a sulfur absorber material and a chromium absorber material, the sulfur and chromium absorber materials having different chemical compositions from one another, the combination of the absorber materials resulting in an irreversible binding of hexavalent gaseous chromium into a solid form within the component, the chromium absorber material being arranged in direct contact with the bulk portion and the sulfur absorber material. The sulfur absorber material and the chromium absorber material may form detectably discrete layers. The chromium absorber may be sandwiched between the bulk portion and the sulfur absorber. The sulfur absorber and the chromium absorber may be located on the bulk portion in an alternating order. The sulfur absorber may form a zone upstream of the chromium absorber. The sulfur absorber may include a carbonate or an oxide having formula (I):

$\text{M}_x\text{A}_z\text{O}_y$  (I),

where

M is an alkaline earth metal or alkali metal,

A is C or Cr,

x is any number between 1 and 3,

y is any number between 1 and 4,

z is any number between 0 and 1.

[0008] The sulfur getter material may include  $\text{CaO}$ ,  $\text{MgO}$ ,  $\text{CaCO}_3$ ,  $\text{MgCO}_3$ ,  $\text{CaCrO}_4$ ,  $\text{MgCrO}_4$ ,  $\text{MgCr}_2\text{O}_4$ , or their combination, and the chromium getter material includes  $\text{BaO}$ ,  $\text{SrO}$ ,  $\text{BaCO}_3$ ,  $\text{SrCO}_3$ ,  $\text{BaCrO}_4$ ,  $\text{SrCrO}_4$ , or their combination.

[0009] In yet another embodiment, a method of resisting release of hexavalent gaseous chromium from a chromium getter material is disclosed. The method may include forming a synergistic combination of getter materials to ensure irreversible binding of gaseous hexavalent chromium within a SOFC system by providing a chromium getter material within the system, upstream from a cathode and providing a sulfur getter material within the system, adjacent the chromium getter material; and providing air to the system, increasing a temperature of the air, and contacting the air with the chromium getter and the sulfur getter such that the chromium getter absorbs gaseous hexavalent chromium into a solid form and the sulfur getter absorbs sulfur-containing gaseous species into a solid form to prevent a reaction of the sulfur-containing gaseous species with the chromium absorbed into the chromium getter. The resisting may be operative throughout the SOFC system lifetime. The method may also include arranging the sulfur getter upstream from the chromium getter. The forming of the synergistic combination may include providing a chromium getter of a different chemical composition than the sulfur getter. The method may also include arranging the chromium and sulfur getter material downstream from a heat exchanger.

[0010] In another embodiment, a method of reducing release of chromium from an electrochemical system is disclosed. The method may include binding chromium-containing molecules from an airstream to a chromium getter material of an electrochemical system component while operating the electrochemical system to obtain bound chromium-containing molecules, the chromium getter material including a saturated state and an unsaturated state through at least a portion of a thickness of the chromium getter material and treating the chromium getter material in the saturated state to reduce contact of the bound chromium-containing molecules in the chromium getter material with the airstream. The chromium getter material in the saturated state has a surface portion and a bulk portion. The treating may include diffusing at least a portion of the bound chromium-containing molecules from the surface portion to the bulk portion by increasing a temperature of the chromium

getter material in the saturated state above an operating temperature and lowering a relative humidity and an oxygen partial pressure below a relative humidity operating value and an oxygen partial pressure operating value, respectively. The method may also include lowering the temperature of the chromium getter material, increasing the relative humidity, and increasing the oxygen partial pressure to the operating temperature, the relative humidity operating value, and the oxygen partial pressure operating value, respectively, when a predetermined unsaturated concentration is reached. The chromium getter material may have a surface portion and a bulk portion and wherein the treating includes applying an amount of an overlay material adjacent the surface portion. The amount of the overlay material may have a same chemical composition as the chromium getter material of the surface portion. The overlay material may be a non-chromium getter material. The non-chromium getter material may include a chromium-free material. The electrochemical system component may be an oxygen outlet component.

[0011] In yet another embodiment, an electrochemical system component of an electrochemical system is disclosed. The component may include a structural ceramic or metal portion; a chromium getter material including an unsaturated surface layer; an unsaturated bulk portion; and a saturated middle layer disposed between the unsaturated surface layer and the unsaturated bulk portion, the saturated middle layer being free of a contact with an airflow in the electrochemical system component. The electrochemical system may be an electrolyzer. The electrochemical system component may be an oxygen outlet component. The system may also include a sulfur getter material separate from the chromium getter material. The unsaturated surface layer may have a same chemical composition as the unsaturated bulk portion.

[0012] In at least one embodiment, an electrochemical chromium monitoring system comprising is disclosed. The system may include a controller programmed to monitor a concentration of chromium in a first chromium getter material portion of a first piping component of the electrochemical chromium monitoring system; redirect an airflow to a second piping component having a second chromium getter material portion when a predetermined saturation level of the first chromium getter material portion is detected, calculated, or projected; and transmit signals to treat the saturated first chromium getter material portion to achieve a predetermined unsaturated concentration of the first chromium getter material portion. The saturated first chromium getter material has a surface portion and a bulk portion. The treating may include diffusing at least a portion of the bound chromium-containing molecules from the surface portion to the bulk portion by increasing a temperature of the first saturated chromium getter material above an operating temperature and lowering a relative humidity and an oxygen partial pressure below a relative humidity operating value and an oxygen partial pressure operating value, respectively. The second chromium getter material portion may have a lower concentration of chromium than the first chromium getter material. The treating may include applying an additional amount of an unsaturated chromium getter material over the first chromium getter material portion. The additional amount of the unsaturated chromium getter material may have a same chemical composition as the first chromium getter material portion. The treating may include applying a layer of a non-chromium getter material onto the first chromium getter material portion. The electrochemical chromium monitoring system may be an electrolyzer.

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## Description

### BRIEF DESCRIPTION OF THE DRAWINGS

[0013] FIG. 1 is a schematic depiction of a non-limiting example of a SOFC;

[0014] FIG. 2 is a schematic example of a SOFC stack;

[0015] FIG. 3A is a schematic depiction of reactions of a traditional SOFC Cr getter material in the beginning of life and middle/end of life of the SOFC system;

[0016] FIG. 3B is a schematic depiction of a non-limiting example of herein-disclosed first and

second getter materials in the beginning of life and middle/end of life of the SOFC system;  
[0017] FIG. 3C is a schematic depiction of an alternative non-limiting example of herein-disclosed first and second getter materials in the beginning of life and middle/end of life of the SOFC system;  
[0018] FIG. 4A is a schematic depiction of a non-limiting example SOFC system including a component having a surface portion including the first/second getter materials disclosed herein;  
[0019] FIG. 4B is a schematic depiction of an alternative non-limiting example SOFC system including a component having a surface portion including the first/second getter materials disclosed herein;

[0020] FIGS. 5A-5D are schematic depictions of non-limiting example arrangements of the first and second getter materials within the component of the SOFC system disclosed herein;

[0021] FIG. 6A is a scatterplot summarizing results of Screening 1 of the Experimental section regarding getter material candidates;

[0022] FIG. 6B is a decision tree analysis showing results relating to the scatterplot of FIG. 6A;

[0023] FIG. 7A is a scatterplot summarizing results of Screening 2 of the Experimental section regarding getter material candidates;

[0024] FIGS. 7B and 7C are a decision tree analysis showing results relating to the scatterplot of FIG. 7A;

[0025] FIG. 8A is a scatterplot summarizing results of Screening 3 of the Experimental section regarding getter material candidates;

[0026] FIGS. 8B and 8C are a decision tree analysis showing results relating to the scatterplot of FIG. 8A;

[0027] FIG. 9 is a plot of reaction probability of SO.sub.x species with various getter compounds identified in the screenings of the Experimental section;

[0028] FIG. 10 show a non-limiting example of a schematically depicted electrolyzer;

[0029] FIG. 11A shows a schematic depiction of a non-limiting treatment of a getter material in a saturated state;

[0030] FIG. 11B shows a schematic depiction of another non-limiting treatment of a getter material in a saturated state;

[0031] FIG. 12 shows a schematic depiction of another non-limiting treatment of a getter material in a saturated state;

[0032] FIG. 13 shows a schematic depiction of a non-limiting treatment of a getter material in a saturated state; and

[0033] FIG. 14 shows a schematic depiction of another non-limiting treatment of a getter material in a saturated state.

#### DETAILED DESCRIPTION

[0034] Embodiments of the present disclosure are described herein. It is to be understood, however, that the disclosed embodiments are merely examples and other embodiments may take various and alternative forms. The figures are not necessarily to scale; some features could be exaggerated or minimized to show details of particular components. Therefore, specific structural and functional details disclosed herein are not to be interpreted as limiting, but merely as a representative basis for teaching one skilled in the art to variously employ the present embodiments. As those of ordinary skill in the art will understand, various features illustrated and described with reference to any one of the figures may be combined with features illustrated in one or more other figures to produce embodiments that are not explicitly illustrated or described. The combinations of features illustrated provide representative embodiments for typical applications. Various combinations and modifications of the features consistent with the teachings of this disclosure, however, could be desired for particular applications or implementations.

[0035] Except in the examples, or where otherwise expressly indicated, all numerical quantities in this description indicating amounts of material or conditions of reaction and/or use are to be understood as modified by the word “about” in describing the broadest scope of the disclosure.

Practice within the numerical limits stated is generally preferred. Also, unless expressly stated to the contrary: percent, “parts of,” and ratio values are by weight; the description of a group or class of materials as suitable or preferred for a given purpose in connection with the disclosure implies that mixtures of any two or more of the members of the group or class are equally suitable or preferred; description of constituents in chemical terms refers to the constituents at the time of addition to any combination specified in the description, and does not necessarily preclude chemical interactions among the constituents of a mixture once mixed.

[0036] The first definition of an acronym or other abbreviation applies to all subsequent uses herein of the same abbreviation and applies mutatis mutandis to normal grammatical variations of the initially defined abbreviation. Unless expressly stated to the contrary, measurement of a property is determined by the same technique as previously or later referenced for the same property.

[0037] It must also be noted that, as used in the specification and the appended claims, the singular form “a,” “an,” and “the” comprise plural referents unless the context clearly indicates otherwise. For example, reference to a component in the singular is intended to comprise a plurality of components.

[0038] As used herein, the term “substantially,” “generally,” or “about” means that the amount or value in question may be the specific value designated or some other value in its neighborhood. Generally, the term “about” denoting a certain value is intended to denote a range within  $\pm 5\%$  of the value. As one example, the phrase “about 100” denotes a range of  $100 \pm 5$ , i.e. the range from 95 to 105. Generally, when the term “about” is used, it can be expected that similar results or effects according to the disclosure can be obtained within a range of  $\pm 5\%$  of the indicated value. The term “substantially” may modify a value or relative characteristic disclosed or claimed in the present disclosure. In such instances, “substantially” may signify that the value or relative characteristic it modifies is within  $\pm 0\%$ ,  $0.1\%$ ,  $0.5\%$ ,  $1\%$ ,  $2\%$ ,  $3\%$ ,  $4\%$ ,  $5\%$  or  $10\%$  of the value or relative characteristic.

[0039] It should also be appreciated that integer ranges explicitly include all intervening integers. For example, the integer range 1-10 explicitly includes 1, 2, 3, 4, 5, 6, 7, 8, 9, and 10. Similarly, the range 1 to 100 includes 1, 2, 3, 4 . . . 97, 98, 99, 100. Similarly, when any range is called for, intervening numbers that are increments of the difference between the upper limit and the lower limit divided by 10 can be taken as alternative upper or lower limits. For example, if the range is 1.1. to 2.1 the following numbers 1.2, 1.3, 1.4, 1.5, 1.6, 1.7, 1.8, 1.9, and 2.0 can be selected as lower or upper limits.

[0040] In the examples set forth herein, concentrations, temperature, and reaction conditions (e.g., pressure, pH, flow rates, etc.) can be practiced with plus or minus 50 percent of the values indicated rounded to or truncated to two significant figures of the value provided in the examples. In a refinement, concentrations, temperature, and reaction conditions (e.g., pressure, pH, flow rates, etc.) can be practiced with plus or minus 30 percent of the values indicated rounded to or truncated to two significant figures of the value provided in the examples. In another refinement, concentrations, temperature, and reaction conditions (e.g., pressure, pH, flow rates, etc.) can be practiced with plus or minus 10 percent of the values indicated rounded to or truncated to two significant figures of the value provided in the examples.

[0041] As used herein, the term “and/or” means that either all or only one of the elements of said group may be present. For example, “A and/or B” means “only A, or only B, or both A and B”. In the case of “only A,” the term also covers the possibility that B is absent, i.e. “only A, but not B”.

[0042] It is also to be understood that this disclosure is not limited to the specific embodiments and methods described below, as specific components and/or conditions may, of course, vary.

Furthermore, the terminology used herein is used only for the purpose of describing particular embodiments of the present disclosure and is not intended to be limiting in any way.

[0043] The term “comprising” is synonymous with “including,” “having,” “containing,” or “characterized by.” These terms are inclusive and open-ended and do not exclude additional,

unrecited elements or method steps.

[0044] The phrase “consisting of” excludes any element, step, or ingredient not specified in the claim. When this phrase appears in a clause of the body of a claim, rather than immediately following the preamble, it limits only the element set forth in that clause; other elements are not excluded from the claim as a whole.

[0045] The phrase “consisting essentially of” limits the scope of a claim to the specified materials or steps, plus those that do not materially affect the basic and novel characteristic(s) of the claimed subject matter.

[0046] With respect to the terms “comprising,” “consisting of,” and “consisting essentially of,” where one of these three terms is used herein, the presently disclosed and claimed subject matter can include the use of either of the other two terms.

[0047] The term “one or more” means “at least one” and the term “at least one” means “one or more.” The terms “one or more” and “at least one” include “plurality” as a subset.

[0048] The description of a group or class of materials as suitable for a given purpose in connection with one or more embodiments implies that mixtures of any two or more of the members of the group or class are suitable. Description of constituents in chemical terms refers to the constituents at the time of addition to any combination specified in the description, and does not necessarily preclude chemical interactions among constituents of the mixture once mixed. First definition of an acronym or other abbreviation applies to all subsequent uses herein of the same abbreviation and applies mutatis mutandis to normal grammatical variations of the initially defined abbreviation. Unless expressly stated to the contrary, measurement of a property is determined by the same technique as previously or later referenced for the same property.

[0049] Fuel cells, or electrochemical cells, that convert chemical energy of a fuel (e.g. H.sub.2 and also other types of hydrocarbons for SOFCs) and an oxidizing agent into electricity through a pair of electrochemical half (redox) reactions, have become an increasingly popular alternative to traditional batteries. Several different types of fuel cells have been developed to cover applications such as automotive, portable power systems, smartphones, combined heat and power, or backup power generation.

[0050] High temperature electrochemical cells, such as those having operating temperature between about 500 and 1000° C., have several advantages over other types of fuel cells. Example high temperature electrochemical cells may be SOFCs and MCFCs. One such advantage is fuel flexibility of the SOFC. For example, a SOFC may reform methane or use carbon monoxide as a fuel. A SOFC may also better tolerate fuel impurities such as ammonia and chlorides. Sulfur-bearing contaminants, though, remain to be problematic. Additionally, the SOFC cathode reaction is heat-absorbing, thus tending to cool the cell down, which may reduce the need for cooling air.

[0051] High temperature electrochemical cells typically feature a relatively high combined heat and power efficiency, long-term stability, fuel flexibility, low emissions, and low cost. High temperature electrochemical cells may operate in temperature ranges of about 750 to 1300 K or about 500 to 1000° C., which may lead to accelerated reactions, but the high temperature may trigger a faster degradation of the components and subcomponents such as interconnects, electrodes, and others. The degradation of the high temperature electrochemical cell components and subcomponents may in turn lead to a drop of the overall cell performance in its lifetime.

[0052] SOFCs are devices which produce electricity directly from oxidizing a fuel. Since fuel cells are characterized by their electrolyte material, the SOFC relates to solid oxide or ceramic electrolyte. A schematic depiction of a non-limiting example of a SOFC is in FIG. 1. As can be seen in FIG. 1, the cell **100** includes an anode **102**, an electrolyte **104**, and a cathode **106**. The cell **100** is provided pure hydrogen as fuel at point A on the anode side and air at point B on the cathode side. In another embodiment, other type of hydrocarbons such as methane may be used at point A in the cell **100**. At the cathode, oxygen present in the air combines with electrons to form oxygen ions, which diffuse through the electrolyte. At the anode, the ions combine with hydrogen to form water.

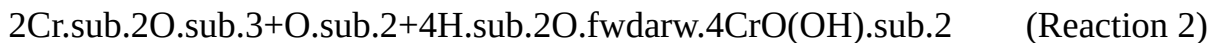
The additional electrons released in the reaction are diverted to produce electricity. Excess fuel and water leave the cell at point C on the anode side and unused gases are expelled out at point D on the cathode side. The cells such as the cell depicted in FIG. 1 are typically combined into stacks to provide a desired amount of voltage.

[0053] A non-limiting schematic depiction of a portion of a SOFC stack **110** is depicted in FIG. 2. As can be seen, FIG. 2 shows spatial distribution of the anode **102**, electrolyte **104**, and the cathode **106** as well as an interconnect **108** within the SOFC cells and the stack. The interconnect **108** is a SOFC component which is in contact with both the anode **102** and the cathode **106**. The interconnect **108**, and other components, face a number of challenging environmental conditions in a SOFC stack. For example, the presence of O<sub>2</sub>/air at the cathode side brings on corrosive conditions which may negatively influence the SOFC components. If the components were not protected, the components' surfaces could suffer from undesirable corrosion and/or metal evaporation.

[0054] The components are typically made from a metal. The metal is typically a steel. The steel may be stainless steel. Ferrous materials such as steel may be naturally passivated by surface oxides, also known as rust, including Fe<sub>2</sub>O<sub>3</sub> and several other metal oxide species. Steel is one of most commonly used materials to fabricate fuel cell components such as PEMC bipolar plate, SOFC interconnect, end plate, gas storage tank, pipe, valve, etc.

[0055] To prevent or lessen the degree of corrosion, high chromium steels with Cr in excess of 12 wt. % have been used because an addition of Cr to a steel composition gives rise to formation of a desirable chromium oxide surface film which provides corrosion resistance to the stainless steel. Preserving the Cr content within the subcomponent may thus contribute to a prolonged cell lifetime by improving corrosion resistance. To achieve preservation of the Cr content, various coatings have been developed. For example, the coatings may include Co<sub>3</sub>O<sub>4</sub> spinel. The coatings may reduce outward diffusion of Cr or help with reducing oxidation rate for steel the component is made from.

[0056] High chromium steels such as 1.4509, AISI 441, X2CrTiNb18 steel may contain about 18 wt. % of Cr. Such stainless steel typically has Cr<sub>2</sub>O<sub>3</sub> oxide materials at the surface. During the high temperature operation of an electrochemical system, Cr<sub>2</sub>O<sub>3</sub> may react with oxygen (O<sub>2</sub>) and/or water (H<sub>2</sub>O) that may form chromium vapors as described in Reactions 1-3 below:



[0057] These Cr vapors, namely, CrO<sub>3</sub>, CrO(OH)<sub>2</sub>, and CrO<sub>2</sub>(OH)<sub>2</sub>, may further react with oxide materials (e.g., cathode) in various cell components that may further poison and thus reduce the fuel cell longevity, performance, or both. For example, the Cr vapors may lead to cathode degradation which may affect long-term stability of the fuel cell stacks.

[0058] The chromium content of the cells has been preserved with materials utilized to prevent chromium entering the cathode and poisoning it, especially at elevated temperatures. Such materials have typically been implemented at the location B within the cell, shown in FIG. 1.

[0059] Among the materials is SrNiO<sub>x</sub>-coated Al<sub>2</sub>O<sub>3</sub> fiber which functions as a "chromium getter" material. A "chromium getter" material relates to a material which may capture the undesirable chromium vapors so that chromium present in the fuel cell system does not reach the stack, and does not increase degree of cathode and/or other degradation. Similarly, SrCoO<sub>3</sub> has been identified as a chromium getter. But both materials have limitations such as toxicity due to presence of Co or Ni. Additionally, the materials' performance and effectiveness need improvement.



Hence, the materials in their known form may not be the most suitable for high temperature electrochemical cell applications.

[0060] Yet, preservation and capture of the chromium content, especially gases, is important throughout the entire cell and stack, for example also at the cathode and anode exhaust sides, locations C and D in FIG. 1.

[0061] After chromium absorption, chromium saturated getters are exposed over their remaining lifetime to different impurities in the gas stream. Especially gaseous forms of sulfur can enter the SOFC system as impurities in the ambient air, fuel, or by release from other components. Through an exchange reaction at the getter, sulfur exposure of Cr pre-loaded Cr getters might, depending on the material, lead to a release of chromium from the getter. Thus, even low concentrations of sulfur, although not leading directly to significant stack degradation, may lead to release of previously captured chromium, which in turn could extensively degrade the stack.

[0062] For example, sulfur may trigger emission of Cr from a chromium getter such as  $\text{SrCO}_3$  in the middle and end of the system life, as is schematically shown in FIG. 3A. Towards the middle to end of the SOFC system life, the concentration of chromium in the gas phase decreases, while sulfur concentration does not change significantly over the lifetime of the system, which may in turn trigger increased release of Cr which was previously captured by Cr getters. As is shown in FIG. 3A, gaseous  $\text{SO}_x$  triggers formation of  $\text{SrSO}_4$  and release of  $\text{CrO}_2(\text{OH})_2$ , which is known to negatively affect the SOFC cell and system significantly more than sulfur. Thus, with the existing Cr getters, it has been a challenge to stabilize the absorbed impurities throughout the length of SOFC operation and its lifetime, and presence of some chromium getters may trigger release of chromium from the getters after initial operation of the system because the impurities in the air may release Cr previously bound by the getter.

[0063] Thus, there is a need to develop a material and method for preserving Cr content in the solid oxide fuel cell and electrolyzer systems, stabilize and irreversibly absorb impurities within the systems, and prevent sulfur-mediated chromium release within the systems, specifically from chromium getter materials.

[0064] In one or more embodiments disclosed herein, an electrochemical system is disclosed. The system may be a high temperature electrochemical system with an operating temperature of about 500-1000° C. The system may include a SOFC or a cell that converts chemical energy of a fuel and oxidant directly into electrical energy. The system may include a solid oxide electrolyzer or another type of an electrolyzer.

[0065] An electrolyzer is a device that uses electricity to split water ( $\text{H}_2\text{O}$ ) into its basic components: hydrogen ( $\text{H}_2$ ) and oxygen ( $\text{O}_2$ ), through a process called electrolysis. The electrolyzer includes two electrodes, an anode and a cathode, separated by an electrolyte that conducts ions but not electrons. When an electric current is applied, water molecules at the cathode release oxygen ions, hydrogen, and electrons. The ions travel through the electrolyte to the anode, where they combine with electrons to form oxygen gas. The resulting hydrogen may be captured and stored as a clean energy source, and the oxygen can be safely emitted. In contrast to proton exchange membrane (PEM) devices, solid oxide electrolysis requires steam, higher temperatures, and the conductive ions are oxygen, not protons. A non-limiting example of an electrolyzer 300 is shown in FIG. 10. The electrolyzer includes a cathode 302, anode 306, and an electrolyte 304. Steam enters at the cathode, which is negatively charged, and accepts electrons which split water into hydrogen gas and  $\text{O}^{2-}$  ions. At the anode, the oxygen ions are oxidized, generating oxygen gas and releasing electrons, which flow through an external circuit to the cathode. The total reaction is as follows:  $\text{H}_2\text{O} \rightarrow \text{H}_2 + \frac{1}{2}\text{O}_2$ .

[0066] The system may include a stack having at least a first cell and a second cell. The stack may have additional cells, up to several dozens or hundreds of individual cells arranged in the stack. The stack may have a planar geometry, tubular geometry, or modified planar fuel cells design geometry. The stack may include 2, 3, 4, 5, 6, 7, 8, 9, 10, 15, 20, 25, 30, 35, 40, 45, 50, 55, 60, 65, 70, 75, 80,

85, 90, 95, 100, or more cells.

[0067] The system is structured to resist/prevent/mitigate/minimize/reduce release of sulfur-mediated chromium into the stack, resist/prevent/mitigate/minimize/reduce overall gaseous chromium influx into the stack and content of gaseous chromium in the stack/cell/system.

[0068] The system may thus include one or more components having a material including a getter material. The component having the getter material may be the same component which releases Cr, S, or both or a component which does not release Cr, S, or both. The getter is a material that captures an element or compound from gaseous species such as  $\text{SO}_x$  or hexavalent Cr and binds the species into a solid form. The binding may be irreversible. The binding may be provided via sorption, absorption, adsorption, or a combination thereof. A getter may be also called an absorber.

[0069] The getter may include a S getter, a Cr getter, or both. The sulfur getter may not be a chromium getter. The sulfur getter may be a chromium getter at the same time as sulfur getter. The sulfur getter may have preferential affinity towards sulfur rather than chromium. The chromium getter is a material that captures gaseous hexavalent chromium and binds it into a solid form. Non-limiting example materials and their function as sulfur/chromium getters within the SOFC system are schematically shown in FIGS. 3B and 3C and described below.

[0070] The getter material may be included in the system upstream from the stack, cell, cathode of a cell/stack, or both. The getter material may be placed prior to the cathode air stream reaching a cathode within the system. The getter material may be placed in the cathode air stream. The getter material may be placed downstream from a heat exchanger, one or more filters, cold air inlet, or a combination thereof. The getter material may be placed within one or more components of the hotbox or the high temperature components of the SOFC system. The hotbox may integrate such components into one unit. An example component may be a pipe, tube, duct, lead, line, canal, channel, carrier, conduit, conveyer, main, or vent leading hot air from a heat exchanger into the stack. The component may be a gas carrying component, gas path component. A schematic depiction of a non-limiting example SOFC system is shown in FIGS. 4A and 4B.

[0071] A non-limiting example SOFC system **200** is shown in FIG. 4A. The system **200** includes the hotbox **208**. The system **200** includes a stack **202** with a fuel inlet **204** and water vapor outlet **206**. The system **200** may include a cold air inlet **210**, a filter **212**, a heat exchanger **214**, a pipe **216** leading the hot air from the heat exchanger **214** to the stack **202**. The system **200** may include a different component structured differently than the depicted pipe **216** leading air of elevated temperature from the heat exchanger **214** to the stack **202**. The component **216** may include the getter or absorber material **218** disclosed herein. In a fuel cell, the component including a getter material may be an outlet component.

[0072] In a system including an electrolyzer, the getter material may be placed on or within one or more components such as a honeycomb structure, metallic component, ceramics, composites, etc. The component may be an inlet or outlet component, for example an oxygen outlet component **316**, schematically shown in FIG. 10.

[0073] The hot box **208** and/or component **216** in a fuel cell, and/or a component **316** in the electrolyzer, may include a bulk material **217**. The bulk material may include steel. The electrochemical cell or system disclosed herein may include a first component, which may include steel and a different, second non-steel component which includes one or more getter materials, as described herein. The steel may be a stainless steel. The steel may be a high chromium steel due to its high electronic conductivity, corrosion resistance, and machinability. The steel may have Cr content of about or at least about 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, or more wt. %, based on the total weight of the steel. The stainless steel may be a stainless steel having a composition SS **304**, SS **316**, SS **316L**, AISI 441, or the like.

[0074] SS **304** contains about 18 wt. % Cr and about 8 wt. % nickel (Ni), while SS **316** contains about 16% Cr, about 10 wt. % Ni, and about 2 wt. % molybdenum (Mo). The difference between

SS **316** and SS **316L** stainless steel is that **316L** has about 0.03 wt. % max carbon (C) and is good for welding whereas SS **316** has a mid-range level of C. The stainless steel may include Cr, Ni, Mo, and/or other elements such as carbon (about 0.03 wt. %), manganese (about 1 to 2wt. %), silicon (about 0.5 to 2 wt. %), nitrogen (about 0.01 to 0.1 wt. %), copper (about 0.5 to 2 wt. %), and cobalt (less than about 0.5 wt. %), where the balance is iron (Fe).

[0075] A non-limiting example composition of AISI 441 used in a high temperature electrochemical cell component may be: C (about 0.03 wt. %), Cr (about 17.5 to 19.5 wt. %), Ni, Mn, Si (about 1 wt. % each), N, S (about 0.03 wt. % each), P (about 0.04 wt. %), Ti (about 0.1 to 0.3 wt. %), Nb (about 0.57 to 0.90 wt. %), where the balance is Fe (about 77 wt. %). The steel may be AISI 441 steel with the chemical formula in mol. %:

Fe.sub.75.6Cr.sub.19.4Si.sub.1.9MnNi.sub.0.9Nb.sub.0.4Ti.sub.0.3C.sub.0.1N.sub.0.1P.sub.0.1S.sub.0.1.

[0076] The steel may be a low chromium steel having content of Cr less than about, at most about, no more than about 10, 9, 8, 7, 6, 5, 4, 3, 2, or 1 wt. %. The cell/stack may include a carbon steel with trace amounts of Cr. The carbon steel may include about, at least about, or at most about 0.02 to 2.1, 0.14 to 0.84, or 0.59 to 0.65 wt. % of C, Mn of about, at most about, or no more than about 0.3 to 1.65, 0.4 to 0.96, or 0.6 to 1.2 wt. %, Si of up to about 0.6 wt. %, and Cu of up to about 0.6 wt. %. The steel may be substantially free of Cr, Ni, Co, Ti, Nb, and/or Mo. The steel may include trace amounts of one or more of the elements named herein.

[0077] The bulk material may include non-steel metals such as aluminum-based material, for example aluminum chromium alloy. The bulk material may include nickel-based alloys, ceramic, or combination thereof.

[0078] The component **216** may include a surface portion **218**. The surface portion **218** relates to a layer or film adjacent to the top of the metallic bulk portion. The surface portion may be immediately adjacent to the top of the metallic bulk portion. The layer or film may be continuous or discontinuous. The layer or film may have the same or different thickness across the area covering the bulk material. The layer or film may include at least one, more than one or one layer or film.

[0079] The surface portion may include one or more compositions structured as a getter material. The getter material may include a first getter material and a second getter material. The first and second getter materials may differ by their chemical composition, chemical, physical, mechanical properties, or a combination thereof.

[0080] The first getter material may be a sulfur getter or sulfur and chromium getter. The first getter material may be sulfur-only getter or sulfur-and-chromium getter. In other words, the first getter material may be structured to reduce/minimize/eliminate gaseous sulfur species such as SO<sub>x</sub> in the air upstream from the stack, in the air entering the stack, and the air in the stack within the SOFC system. The first getter material may thus prevent formation of chromium species in the hot air stream upstream from the stack, prevention of which is achieved by chemical interaction between sulfur-based impurities in the incoming air stream and the first getter material chemistry.

[0081] The first getter material may have affinity towards sulfur such that sulfur binds, reacts, sorps, absorbs, or adsorbs to the first getter material. The binding, reaction, sorption, absorption, adsorption refers to a substantial fraction of the gaseous species attaching to the first getter material such that the species are no longer in the gaseous form, being prevented from damaging the stack. Gibbs free energy change of the absorption process, which is targeted to be negative (i.e. thermodynamically preferred), may be used to measure the binding.

[0082] The first getter material may have affinity towards chromium as well as sulfur. The affinity towards chromium may be lower than affinity towards the sulfur.

[0083] The binding, sorption, absorption, adsorption may be irreversible such that the sulfur is bound for an extended period of time. The extended period of time may be up to lifetime of the system. The first getter material may include one or more compositions disclosed herein. The first getter material may include a mixture of compositions. The amount of individual compositions within the first getter material may be equal or different.

[0084] The sulfur getter material/surface portion may be arranged to react with one or more sulfur vapor species present in the air passing via the hotbox **208** and/or component **216**. The sulfur vapors may include SO.sub.x and other gaseous sulfur-containing species, including, but not limited to, H.sub.2S, H.sub.2SO.sub.4, SO, SO.sub.2, SO.sub.3, C.sub.2H.sub.6S, C.sub.2H.sub.6OS, COS, and/or CS.sub.2. The expression SO.sub.x within this disclosure relates to any and all sulfur-containing gaseous species named herein. The chromium getter material/surface portion may be structured to form and/or have stable interface with the bulk material.

[0085] The getter material may include a second getter material. The second getter material may include a chromium getter material. The chromium getter material may not be a sulfur getter material. In other words, the second getter material may not have affinity towards sulfur and may not be structured to bind, sorp, absorb, or adsorb sulfur from the air/fluid present in the component or system. The second getter material may be chromium-only getter. The second getter material may be a chromium absorber.

[0086] The Cr getter material may have 3 states: (1) an empty state, for example SrCO.sub.3 prior to its reaction with gaseous Cr, (2) a thermodynamically preferred Cr-rich state or Cr getter state, for example when exposed to gaseous hexavalent chromium CrO.sub.2(OH).sub.2, CO.sub.2 and H.sub.2O is released, and SrCrO.sub.4 is formed, and (3) a sulfur-rich and/or nitrate-rich state, for example when SrCrO.sub.4 is exposed to SO.sub.x species and H.sub.2O, SrSO.sub.4 may be formed and CrO.sub.2(OH).sub.2 may be released. Since Cr is significantly worse than S with respect to SOFC stack degree of poisoning, state (3) leads to aggravated stack degradation and decrease of lifetime in SOFCs.

[0087] Hence, state (3) is the state during which the previously bound hexavalent Cr is re-released into the cathode air stream and potentially leads to degradation of the stack. To prevent realization of state (3) of the Cr getter within the system, the first getter is included. Presence of the combination of the first and second getter material together allows for an irreversible absorption of Cr impurities as there is no thermodynamic driving force to release the initially absorbed air impurity (hexavalent Cr within the Cr getter), leading to a higher absorption efficiency over the lifetime of the SOFC system. Subsequently, this leads to a longer lifetime while preserving stack performance for longer. The first and second getter materials thus cooperate and work synergically to prevent degradation of the SOFC stack.

[0088] The chromium getter material/surface portion may be arranged to react with one or more chromium vapor species present in the air passing via the hotbox **208** and/or component **216**. The chromium vapors may include Cr—O—(H) species, including, but not limited to, CrO, CrO.sub.3, CrO.sub.3H.sub.2, CrO.sub.4H.sub.2, and/or CrO.sub.3O.sub.2. The chromium getter material/surface portion may be structured to form and/or have stable interface with the bulk material.

[0089] The first getter material, second getter material, or both may include a carbonate, oxide, or both. The first and/or second getter material may include an alkaline earth metal. The second getter material may include Be, Mg, Ca, Sr, or Ba. The first and/or second getter material may include, comprise, consist essentially of, or consist of at least one or one or more compounds having a general formula (I):

M.sub.xA.sub.zO.sub.y (I),

where

M is an alkaline earth metal or alkali metal,

A is C or Cr,

x is any number between 1 and 3,

y is any number between 1 and 4,

z is any number between 0 and 1.

[0090] In the formula (I), M may be, Mg, Ca, Sr, Ba, or Li.

[0091] In the formula (I), A may be absent, A may be C or Cr.

[0092] In the formula (I), x may be 1, 1.1, 1.2, 1.3, 1.4, 1.5, 1.6, 1.7, 1.8, 1.9, 2.0, 2.1, 2.2, 2.3, 2.4, 2.5, 2.6, 2.7, 2.8, 2.9, or 3.0. In the formula (I), y may be 1, 1.1, 1.2, 1.3, 1.4, 1.5, 1.6, 1.7, 1.8, 1.9, 2.0, 2.1, 2.2, 2.3, 2.4, 2.5, 2.6, 2.7, 2.8, 2.9, 3.0, 3.1, 3.2, 3.3, 3.4, 3.5, 3.6, 3.7, 3.8, 3.9, or 4.0. In the formula (I), z may be 0, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, or 1.0. If z is 1, y may be 3.

[0093] Non-limiting example compounds of formula (I) include BeO, MgO, CaO, SrO, BaO, BeCO.sub.3, MgCO.sub.3, CaCO.sub.3, SrCO.sub.3, BaCO.sub.3, CaCrO.sub.4, MgCrO.sub.4, MgCr.sub.2O.sub.4, BaCrO.sub.4, or SrCrO.sub.4.

[0094] The first and/or second getter material may include, comprise, consist essentially of, or consist of at least one or one or more phosphates, silicates, or both having a general formula (II):

Li.sub.aA.sub.bM.sub.xO.sub.y (II),

where

A is a transition metal,

M is a metalloid or reactive non-metal,

a is any number between 1 and 4,

b is any number between 0 and 2,

x is any number between 0.1 and 3,

y is any number between 1 and 6.

[0095] In the formula (II), A may be Fe, Cr.

[0096] In the formula (II), M may be Si or P.

[0097] In the formula (II), a may be 1, 1.1, 1.2, 1.3, 1.4, 1.5, 1.6, 1.7, 1.8, 1.9, 2.0, 2.1, 2.2, 2.3, 2.4, 2.5, 2.6, 2.7, 2.8, 2.9, 3.0, 3.1, 3.2, 3.3, 3.4, 3.5, 3.6, 3.7, 3.8, 3.9, or 4.0. In the formula (II), b may be 1, 1.1, 1.2, 1.3, 1.4, 1.5, 1.6, 1.7, 1.8, 1.9, or 2.0. In the formula (I), x may be 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1, 1.1, 1.2, 1.3, 1.4, 1.5, 1.6, 1.7, 1.8, 1.9, 2.0, 2.1, 2.2, 2.3, 2.4, 2.5, 2.6, 2.7, 2.8, 2.9, or 3.0. In the formula (I), y may be 1, 1.1, 1.2, 1.3, 1.4, 1.5, 1.6, 1.7, 1.8, 1.9, 2.0, 2.1, 2.2, 2.3, 2.4, 2.5, 2.6, 2.7, 2.8, 2.9, 3.0, 3.1, 3.2, 3.3, 3.4, 3.5, 3.6, 3.7, 3.8, 3.9, 4.0, 4.1, 4.2, 4.3, 4.4, 4.5, 4.6, 4.7, 4.8, 4.9, 5.0, 5.1, 5.2, 5.3, 5.4, 5.5, 5.6, 5.7, 5.8, 5.9, or 6.0.

[0098] Non-limiting example compounds of formula (II) include Li.sub.2Fe(SiO.sub.3).sub.2 or LiFePO.sub.4.

[0099] The first getter material may include, comprise, consist essentially of, or consist of one or more ionic liquids, metal salts, or both. The first getter material may include, comprise, consist essentially of, or consist of one or more compositions structured to absorb or convert NO<sub>x</sub> such as a platinum-group-metal catalytic converter.

[0100] The second getter material may include one or more compositions including one or more conventional Cr getter compositions that are already known, such as alkaline earth oxides, alkaline earth carbonates, transition metal oxides, or a combination thereof.

[0101] The getter materials may include a mixture or combination of the compositions disclosed herein such that the mixture may include 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, or more compositions within at least one or in each getter layer/zone/material.

[0102] In one or more non-limiting example embodiments, the first getter material includes CaO, MgO, CaCO.sub.3, MgCO.sub.3, or their combination, and the second getter material includes BaO, SrO, BaCO.sub.3, SrCO.sub.3, or their combination. In another non-limiting example embodiments, the first getter material may include Li.sub.2Fe(SiO.sub.3).sub.2 or LiFePO.sub.4, or both, and the second getter material may include BaO, SrO, BaCO.sub.3, SrCO.sub.3, or their combination. In yet another non-limiting example, the first getter material may include MgO, a metal salt, and the second getter material may include SrCO.sub.3. In yet another non-limiting example, the first getter material may include CaO and MgO, and the second getter material may include SrCO.sub.3 and BaCO.sub.3.

[0103] In a non-limiting example, at some point in its lifetime, the system may include a composite

of (Sr,Ba)CrO<sub>2</sub> and (Mg,Ca)O and/or (Mg,Ca)CO<sub>2</sub>. This material is capable of absorbing sulfur without releasing Cr, rather than the conventional SrCrO<sub>2</sub> which may release Cr.

[0104] One or more compounds identified within the formulas (I), (II), may be expressly excluded from the first getter material, second getter material, or both, disclosed herein. The exclusions may be, for example, due to toxicity or environmental concerns.

[0105] The material of formulas (I), (II), or both, may be further modified to include an oxygen vacancy of at least 10% off-stoichiometry to enhance gas diffusion. The materials may thus be off stoichiometric. The getter materials identified herein may be used to react with the identified gaseous species including Cr such as CrO<sub>2</sub>(OH)<sub>2</sub> to lower/minimize/eliminate the concentration of Cr<sub>6+</sub> in the cathode air stream.

[0106] The getter material may include one or more sacrificial compounds incorporated in the cathode air stream. "Sacrificial" relates to a compound that is consumed by the reactions and is not further present in the system in its original chemical form after the reaction(s) the compound is part of take place. The sacrificial compound may be reactive or highly reactive with the hexavalent gaseous species and/or SO<sub>x</sub> species such that any gaseous chromium/SO<sub>x</sub> would be further converted into benign species. The product of the reaction of the sacrificial compound and the gaseous Cr/SO<sub>x</sub> may be stored within the system, component including the sacrificial compound, or both. The product may stay within the system in an irreversibly solid state for a predetermined period of time. The period of time may be or be up to the lifetime of the system. Alternatively, the product, once accumulated within the component, may be removed as part of a replacement process of the component.

[0107] Alternatively, or in addition, the component **216** may include a structure **220** including the getter material. A non-limiting example system with the structure **200** is shown in FIG. 4B. The system **200** depicted in FIG. 4B includes the separate structure **220** within the component **216**. The structure is upstream from the stack **202** and downstream from the heat exchanger **214**. The structure **200** may be a honeycomb, porous, or ceramic structure including a bulk portion, which may be, for example alumina. The porous structure may have pore sizes of about 1 μm-5 cm, 10 μm-500 μm, or 100 μm-200 μm. The porous structure may have pore sizes of about, at least about, or at most about 1, 10, 50, 100, 150, 200, 250, 300, 350, 400, 450, 500, 550, 600, 650, 700, 750, 800, 850, 900, 950, or 1000 μm. The structure may include a surface portion **218** described above. The porous structure may be located in the flow path of the component **216** such that the air influx pushes through the pores of the structure. The relatively high surface area of the structure may assist with the capture of the unwanted species in the air.

[0108] The getter material may be distributed in the component **216** evenly throughout the length, volume, and/or area of the component **216**. Alternatively, the getter material may be accumulated predominantly adjacent to the heat exchanger **214**. At least some portions of the component **216** may be free of the getter material. The getter material may be applied as a washcoat on the bulk portion or on the surface of the honeycomb structure **220**. The washcoat may be provided, for example via solution deposition. The washcoat may be annealed at a temperature at or above about 100° C. to reduce a number of defects in the washcoat.

[0109] The getter material, as the surface portion, may be applied in layers onto the bulk portion. For example, the surface portion may include 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, or more layers of the getter material. Each or at least some of the layers may include both the first and second getter material. The getter material may be mixed within the layers. As a result of such application, each layer may include the first getter material and the second material. The amounts of each getter material may be even or uneven. A non-limiting example of such arrangement can be seen in FIG. 5A, in which the bulk material **217** is schematically shown to carry the surface portion **218** including the first getter material **230** and the second getter materials **232** intermixed with each other or forming a composite.

[0110] Alternatively, the placement of the first and second getter material within the layers may be

specifically designed to achieve a goal of maximizing the amount of poison species capture such as forming a sulfur-getter zone and a chromium-getter zone. Non-limiting example embodiments of the zone layering are shown in FIGS. 5B, 5C, and 5D. The layers may be detectably discreet layers. Since the main concern is lifetime performance of the system, and especially middle and end life of the SOFC system, the getter zones may be designed to combat sulfur-mediated or sulfur-induced chromium release. As such, in the example embodiment of FIG. 5B, the first getter material may be provided in the top layer to preferentially capture the sulfur species to prevent sulfur-mediated chromium release from the second getter material. The surface area of the first getter is thus maximized.

[0111] In the example embodiment depicted in FIG. 5C, as the air influx with impurities encounters the surface portion with the getters, the air first contacts the first getter with S-binding material. Subsequently the air proceeds to the second getter material binding the chromium. The sulfur getter is thus located upstream from the chromium getter. Since the air is free or substantially free from the sulfur gaseous species after interaction with the first getter material, the absorption of chromium into the second getter is irreversible.

[0112] FIG. 5D show a yet another non-limiting example of the zone placement of the first and second getter materials. In the embodiment shown in FIG. 5D, the first and second getter zones alternate such that any sulfur and chromium present in the air influx can be captured within the surface portion. The sulfur getter and the chromium getter are provided in an alternating order/zones.

[0113] A method of resisting/decreasing/minimizing/reducing/eliminating Cr in the inlet air stream/cathode air stream is disclosed herein. The method may include resisting/preventing sulfur-mediated chromium release from a solid source within the system. The resisting of release of the Cr absorbed into the Cr getter may be operative throughout the SOFC system lifetime. The solid source may be a chromium getter previously binding Cr. The method may include incorporating one or more getter materials within the system upstream of a cathode, cell, stack. The method may include utilizing a first getter material as a S getter, capturing one or more gaseous SO<sub>x</sub> species from the air stream downstream from a heat exchanger. The method may include utilizing the first getter material predominantly during the middle and end of the life of the system when the S concentration is increased in comparison with the beginning of life of the system. The method may prevent reaction of a Cr getter material with water and SO<sub>x</sub> species resulting in unwanted release of CrO<sub>2</sub>(OH)<sub>2</sub> from a Cr getter material.

[0114] The method may include utilizing more than one type of a getter material, for example a first getter material which is a S getter or absorber and a second getter material which is a Cr getter or absorber. The method may include providing the first and second getter material in layers, patterns, zones, as was described above.

[0115] The method may include using at least some of the getter materials as sacrificial materials. The method may include binding, sorbing, absorbing, adsorbing, or reacting with hexavalent Cr and/or SO<sub>x</sub> species in a solid form within a component including the getter material(s). The method may include binding the S species, Cr species, or both irreversibly. The method may include preventing release of previously bound Cr from a getter material within the component. The method may also include capturing gaseous Cr species from the air stream prior to the species entering the stack, cell, cathode. The method may include accumulating the SO<sub>x</sub> species, Cr species, in a solid form and retaining the species in their solid form for a period of time which may be up to the lifetime of the system. The method may include replacing a component containing the accumulated species to remove the species from the system, to replenish the getter materials within the system, or both.

[0116] The method may include producing the component including the surface portion having one or more materials of formulas (I), (II), additional material named herein, or a combination thereof. The method may further include manufacturing at least one component having the one or more

compositions disclosed herein. The method may include providing a predetermined amount of the one or more compounds of the formulas (I), (II), additional material named herein, or a combination thereof, in the surface portion on the metallic bulk portion of a component of the system, the component being located upstream from a cathode, cell, stack, or a combination thereof. [0117] The method may include utilizing one or more techniques to deposit the materials of the formulas (I), (II), and/or additional material named herein, or a combination thereof on the component. The method may include washcoating one or more internal surfaces or bulk portion of the component. The method may include providing the disclosed getter materials along the entire surface of the component or portion(s) of the surface of the component. The method may include providing the getter materials in patterns, zones, layer, as described above, with the same or different thickness throughout the application area.

[0118] The method may include forming a separate structure such as a honeycomb structure and washcoating the getter materials onto the structure, in patterns, layers, zones, as was described above. The method may include providing the structure with the getter materials within the component of the system, the structure and component being located upstream of a cathode, cell, stack, or a combination thereof.

[0119] The advantage of the herein-described system lies in elimination/reduction of overall hexavalent chromium entering the stack, thus preventing or reducing chance of stack degradation and increasing its lifetime. Another advantage lies in reducing the chance of reversible Cr binding within the system upstream of the stack via preventing or minimizing sulfur-mediated release of Cr from a Cr getter.

[0120] In one or more embodiments, apparatus and methods for recovery or treatment of a saturated getter material also referred to as a material in a saturated state are disclosed. The saturated getter material or a material in a saturated state relates to a getter material which has been exposed to species it has affinity for, such as Cr, S, etc. and has reached its maximum capacity to bind the species. As a result, the saturated getter does not function as a getter anymore, and the species bypass the getter without binding onto it, or worse emit the bound species via an atom-exchange mechanism. For example, the saturated chromium getter may be exposed to sulfur, allowing a sulfur-chromium exchange mechanism to emit hazardous previously-absorbed chromium to the environment. To enable or renew binding of the species to the getter material, the getter material needs to be treated. The treatment may result in a partially saturated or unsaturated getter material which has a renewed capacity to bind species such as Cr, S, etc. when exposed to the species. A saturated getter material refers to a material which used to bind one or more species such as Cr, S, etc. in the past but which has reached its maximum capacity for binding the species and can no longer bind the species. A partially saturated and unsaturated getter material, also referred to as a material in an unsaturated state, refers to a material capable of binding one or more species such as Cr, S, Cr-containing molecules, S-containing molecules, etc. which has not reached its maximum capacity for binding the species and continues to be able to bind the species. The bound molecules may include additional elements besides the species of interest such as Cr, S, etc.

[0121] The treatment may be carried out during operation of the cell or system. Alternatively, the treatment may be provided when the operation of the cell or system is temporarily interrupted or stopped.

[0122] The saturated getter material may be treated to reach a lower concentration of a species the getter material binds. For example, if Cr is the species, an amount of Cr on a saturated chromium getter may be thus reduced in a controlled manner. Specifically, the concentration of Cr (OH).sub.2O.sub.2 bound to the getter material may be lowered.

[0123] The treatment may include an oxidizing or reducing wash or hot-gas flush, where the wash or gas may include water, alcohol, ethyl acetate, sodium hypochlorite, nonaqueous or other solvent containing oxidizing or reducing additives such as ozone, bleach, chlorine, hydrogen peroxide, hydrides, citric acid, hydrochloric acid, various acids, various bases, or their combination. The



temperature of this process may be varied from ambient conditions up to about 1200° C. The wash or gas flush may result in removal of the bound species/contaminants from the getter material. A schematic depiction of the treatment including a wash or gas flush is shown in FIG. 11A. FIG. 11A shows a system 400, as disclosed herein, including a getter material saturated with chromium 402. The wash or gas flush 404 is applied onto the getter 402 and results in chemical release of the bound species such as chromium 406, which may be subsequently removed from the system 400. The thick arrow indicates the direction of air flow. The thin arrow indicates that after the removal of chromium from the saturated material 402, incoming chromium species in the air flow can again bind to the getter material.

[0124] Alternatively or in addition, the treatment may include heating the saturated getter material in a low-oxygen, low-humidity environment, thereby diffusing the bound species from the surface portion deeper into the bulk portion of the getter material. Removal of the bound species from the surface portion to the bulk portion may thus secure the species within the getter material. The heating in a low-oxygen and low-humidity environment results in the diffusion into the bulk portion and minimizes evaporation of the species such as chromium from the getter material during the heating. The heating may be performed between about 200-1200, 400-1100, or 600-1000° C., depending on the tolerances for species emission during the heating process and the temperature of species absorption. A non-limiting undesirable evaporation reaction of a strontium-based chromium getter includes the following chemical reaction:

$\text{SrCrO}_4 + \text{H}_2\text{O} \rightarrow \text{SrO} + \text{Cr}(\text{OH})_2$ , which requires water or a parallel oxidation reaction that requires oxygen. A low humidity prevents the unwanted evaporation and maximizes the desirable diffusion of bound species into the bulk portion instead.

[0125] In an electrochemical cell, the low humidity refers to humidity lower than a typical humidity during operation for the given cell or system. Under normal operation, the oxygen side of a solid oxide electrochemical cell may have a water concentration of up to about 20%, but more typically 3-10%. The low humidity thus refers to a value lower than the typical humidity of a specific system disclosed herein. The low humidity may thus refer to values of about 20, 19, 18, 17, 16, 15, 14, 13, 12, 11, 10, 9, 8, 7, 6, 5, 4, 3, 2, or 1%. The relative humidity depends on the temperature of operation, so heating above the operating temperature can reduce the relative humidity substantially.

[0126] In an electrochemical cell, the low oxygen partial pressure refers to oxygen levels lower than typical oxygen levels during operation for the given cell or system. A low oxygen level refers to reduced oxygen partial pressure ( $p\text{O}_2$ ) at the cathode of a SOFC fuel cell. Ambient air  $p\text{O}_2$  is about 0.21 atm or 21% of  $\text{O}_2$  in air. Low oxygen conditions may include  $p\text{O}_2$  substantially less than about 0.21 atm such as 0.01, 0.001, or 0.0001 atm. A high-nitrogen gas flow can ensure low oxygen content during the treatment process.

[0127] The low-humidity environment of the system may be achieved by providing a strong water sorbent such as a zeolite, silica, hygroscopic salt, etc. to absorb offgassing water. Alternatively, the low humidity of the system may be achieved by a strong flow of inert gas such as  $\text{N}_2$ .

[0128] A schematic depiction of the treatment is shown in FIG. 11B. FIG. 11B shows a system 400, as disclosed herein, including a getter material 402 having a thickness. The thickness may include a surface portion 401 and a bulk portion 403. The getter material in a saturated state may have a concentration gradient of the bound species such as Cr. The greatest concentration of the bound Cr species may be at the top of the surface portion, gradually decreasing towards the bottom of the surface portion and towards the bulk portion.

[0129] In the non-limiting example of the system 400, the getter material 402 is saturated with the bound species such as chromium in the surface portion 401. The increased temperature, low relative humidity, and reduced oxygen partial pressure is applied onto the getter material 402 and results in diffusion of chromium 406 from the surface portion 401 into the bulk portion 403 of the getter material 402. After the treatment, the getter material in the saturated state, the bulk portion 403, is

free of contact with the airflow.

[0130] The saturated getter material may be also treated with a new deposit or additional amount of the getter material. The new deposit may be a layer or more than one layer deposited over the saturated getter material. The layer(s) may be continuous or discontinuous. The new deposit may be a physically separate material, not a portion of the original getter material. The new deposit provides extra unsaturated getter material which may absorb chromium without sulfur-chromium exchange. In a non-limiting example, a new layer of SrO may be deposited onto a surface portion of the saturated getter material. The deposition may include sputtering, electrodeposition, liquid deposition, or any other suitable method. The new deposition of the getter material may have the same or different chemical composition as the original getter, prior to the getter's binding to the species disclosed herein. A schematic non-limiting example new deposit is shown in FIG. 12. The system **400**, as shown in FIG. 12, includes the getter material saturated with chromium **402** as the bottom layer, and the new deposit including a getter material, unsaturated with chromium, **408**, as the top layer exposed to the airflow, indicated by the thick arrow. The thin arrow indicates that the unsaturated getter portion **408** is capable of binding chromium from the airflow. After the treatment, the getter material in the saturated state is free of contact with the airflow.

[0131] Alternatively, the saturated getter material may be encapsulated instead of treated. Encapsulation may relate to the getter material being sealed off from the exhaust/airflow, thus reducing or minimizing the risk of sulfur-chromium exchange. The saturated material may be thus removed from exposure to the exhaust/airflow while a getter material in an unsaturated state is further available for sorbing the species such as Cr.

[0132] The encapsulation may be provided by physically blocking or coating the saturated portions with a solid material cover such as one or more layers of a material preventing release of chromium. The material may not be a S or Cr getter material. The material may be free of S, Cr, or both. The material may include aluminum, steel, polymer, ceramic, metal, or silicone, or their combination, chosen on the basis of the operating temperature and gas atmosphere of the encapsulated component. The encapsulation may be provided manually or automatically.

[0133] The unsaturated getter material may be an originally deposited material. In other words, the unsaturated getter may be a portion of the original deposit where a portion became saturated with the species such as chromium and a portion remains unsaturated. Such embodiment is depicted schematically in FIG. 13. The system **400** shown in FIG. 13 includes the getter material saturated with chromium **402**, a sealing layer **410**, and the unsaturated portion **412** functioning as the getter material. The thick arrow shows direction of airflow. The thin arrow indicates movement of chromium species towards the unsaturated getter portion **412**.

[0134] The encapsulation may be alternatively provided by redirecting the airflow from one area of the system towards another area of the system, e.g. via valves to direct the flow away from the saturated portions of the getter material. A non-limiting schematic example is shown in FIG. 14. The system **400** includes a plurality of pipes or piping **420**, **422**, each pipe including a chromium getter material. Initially, the air flow may be led through the first pipe **420**, resulting in the first getter material **402** in the first pipe **420** becoming saturated. After saturation of the first getter material, the airflow may be redirected to a second pipe **422**, which includes a second getter material which is unsaturated **412**. The redirection may be facilitated via opening and closing of one or more valves **430** of the system **400**. The first getter material **402** in a saturated state may be treated as disclosed herein, and the now-unsaturated first getter material of the first pipe **420** may be used after the second getter material of the second pipe **422** becomes saturated or at the same time as the second getter material of the second pipe **422**. The switching of the airflow between the pipes, depending on a saturation level of the first and second getter materials, may be coordinated by one or more controllers, as is described herein. The switching may be cyclical, random, or regular.

[0135] The system may include one or more controllers programmed to facilitate the getter material

treatment. The one or more controllers have one or more processing components such as one or more microprocessor units (not depicted) which enable the controllers to process input data from one or more devices, sensors, or a combination thereof. The devices and sensors may include an inlet or outlet stream temperature sensor, inlet or outlet stream airflow velocity, inlet or outlet stream chromium concentration sensor, inlet or outlet stream sulfur concentration sensor, inlet or outlet humidity sensor, a timer, a clock, or their combination. The one or more controllers may be in communication with one another and/or with other portions of the system. A non-limiting schematic depiction of a controller **440** and sensors **442** is shown in FIG. **14** and is only exemplary. Another non-limiting example of a controller **340** and sensors **342** is shown in FIG. **10**. The sensors are located at the outlets in the system **300**.

[0136] The input data supplied from the sensors may include real time electrode inlet and outlet flow rates and temperatures, real time temperature at predetermined measurement locations, concentration of chromium, sulfur, or a combination thereof. At set intervals, the one or more controllers may compare the input signal to a predefined set point or a threshold value. If the input signal deviates from the set point or threshold value, the controller(s) may provide a corrective output signal to one or more portions of the system such as a signal to initiate a treatment of the getter material, as disclosed herein.

[0137] The controller may be programmed to calculate, assess, determine, communicate, initiate, or a combination thereof, treatment of the getter material based on the input. For example, the controller may be programmed to determine the level of chromium saturation based on input from one or more sensors, comparing the input to initial input values, or both. The controller may be programmed, based on the determination, to initiate treatment of the saturated surface layer or portions of the surface layer. The controller may be programmed to start, maintain, and stop a wash or increase temperature, lower oxygen saturation, lower humidity within the system to diffuse chromium from the surface layer to the bulk portion(s) of the getter material.

[0138] The controller may be programmed to indicate, detect, project, calculate, or combination thereof, a predetermined saturation level of the getter material, send signals to stop operation of the system when the predetermined saturation threshold is reached, send signals to restart the system when a detectable concentration of the chromium in the getter material is lower than the threshold value, or a combination thereof.

[0139] The controlled may be programmed with an algorithm. The controller may direct its inputs toward a machine-learning model that is hosted locally or in the cloud. The controller's machine-learning model may be retrained based on input from multiple controllers of a known configuration and their measurements.

[0140] A method of treating a getter material in a saturated state is disclosed. The method may include one or more steps in combination. The method may contribute to minimizing, reducing, mitigating, or eliminating release of chromium from the cell or system disclosed herein. The method may include binding chromium-containing molecules from airstream to a chromium getter material of the cell or system while operating the cell or system. The method may include treating the chromium getter material to prevent contact of the saturated chromium getter material with the airstream, to lower a chromium concentration of the saturated chromium getter material to a predetermined unsaturated concentration of chromium, or both.

[0141] The method may include diffusing chromium molecules from the surface portion of the getter material to the bulk portion of the getter material by increasing temperature of the saturated chromium getter material above an operating temperature, lowering relative humidity below an operating value, lowering oxygen partial pressure below an operating value, or their combination. The method may include preventing evaporation of the species from the getter material by increasing the temperature, lowering relative humidity, lowering oxygen partial pressure, or their combination, to typical operating values and conditions of the system.

[0142] The method may include treating the surface portion of the getter material with an oxidizing

or reducing wash or gas flush to change an oxidation state of the bound species and releasing the species from the getter material. The method may include capturing the released species.

[0143] The method may include preventing a contact or fluid communication between the saturated getter material and airflow in or outside of the cell or system. The method may include applying an additional amount of a material over the surface portion of the getter. The material may be a getter material or a non-getter material. The method may include completely or partially covering or overlaying the getter material in a saturated state with the additional material.

[0144] The method may include monitoring concentration(s) of Cr, S, or both within the getter material, components, cells, systems, or their combination, disclosed herein. The monitoring may be executed by one or more controllers, sensors, other devices, or their combination. The method may include setting, calculating, projecting, detecting, or their combination, a threshold concentration of Cr indicative of the getter material being in a saturated state. The method may include sending signal to treat and treating the getter material based on input from the controller. The method may include redirecting, switching, shifting, diverting, or rerouting airflow from one portion of the cell or system with a getter material in a saturated state to another portion of the cell or system with an getter material in an unsaturated state. The method may include treating the saturated getter material and reusing the treated getter material. The method may include redirecting the airflow based on level of wanted species saturation, time interval, predetermined values, or their combination. The method may include combining one or more treatment methods in one cell, system, or both.

#### Experimental Section

[0145] The one or more oxides of formula (I) were identified using publicly available materials database to screen for the optimal materials, and high-throughput (HT) first-principles density functional theory (DFT) was used to calculate the results to evaluate and identify suitable getters materials.

[0146] The following screening criteria were used: [0147] (a) Total energy of a computed structure (typically in eV/atom or eV) describes the computed energy of a structure; the differences between structures correspond to a reaction energy between those structures. For example, the reaction  $A \rightarrow B$  has a reaction energy  $E_B - E_A$  (where the energies might be written in kJ/mol); [0148] (b) Convex-hull decomposition (or decomposition)—the convex hull of all stable compositions may be constructed such that each chemical composition C has a minimum combination of stable states,  $C \rightarrow A+B$ , where the stoichiometric formula of C is equal to the sum of A and B, and there is no other  $A'+B'$  that has a lower energy. Then A+B is the convex-hull decomposition products of C. If the energy of C is known, then the hull energy or decomposition energy (typically eV/atom or eV) is  $E_h = E_C - E_A - E_B$  and is always a nonnegative number. In some conventions it is reported as the reaction energy  $E_{rxn} = E_A + E_B - E_C$  and is always a nonpositive number.

[0149] The screening-gained information was used to explore various classes of chemicals: known materials whose DFT structure can be computed; typically single-crystal or gas-phase molecules as well as compositional formulas, even if the atomic structure is not known, as long as related structures are available in a database. This includes: adjusting compositional ratios, such as excess oxygen or oxygen vacancies and dopants and substitutions.

[0150] Several properties were computed:

[0151] 1. Stability at a fixed temperature—this can be given by the hull energy; if it is less than the temperature (times the Boltzmann constant  $k_B$ ), then it is stable. Alternatively, it can be computed by the oxygen chemical potential, which can be benchmarked to temperature at a known scale.

[0152] 2. Filtering by atom size, oxidation state, metal-oxygen ratio, crystal structure, spacegroup, elements, etc.

[0153] 3. Elemental material cost, per mol or per kg.

[0154] 4. Reactivity screening, which is the likelihood of a reactivity between the composition C and a reactant R. Using the convex-hull methodology, the reactivity can be computed by examining (1) the decomposition products of a composition  $C+xR$  and (2) the relative decomposition energy of  $\epsilon(x)=E(C+xR)-E(C)-xE(R)$  (a nonpositive number). The most stable reaction is the one that has the minimum  $\epsilon$ , while the dilute limit is the lowest value of  $x$  that has a nonzero  $\epsilon$ .

[0155] Subsequently, the reactivity was benchmarked to a known material  $C'$  using the following two quantities:

[0156] (a) At which molar fraction  $x$  does the reaction occur? A higher reactivity is associated with a higher value of  $x$ , i.e. more of the reaction occurs per molar unit of C (or  $C'$ ). A typical metric here is:  $RR_{\text{sub.stoich}}=x_{\text{sub.C}}/x_{\text{sub.C'}}$ , where  $C'$  is the reference material and  $RR$  stands for the relative reactivity.

[0157] (b) What is the relative decomposition energy  $\epsilon$ ? A higher reactivity is associated with a lower value of  $\epsilon$  (higher absolute value), i.e. the reaction is more energetically favorable. A typical metric here is:  $RR_{\text{sub.en}}=\epsilon_{\text{sub.C}}/\epsilon_{\text{sub.C'}}$ , where  $C'$  is the reference material. It can also be:  $RR_{\text{sub.en}}=(\epsilon_{\text{sub.C'}}-\epsilon_{\text{sub.C}})/k_{\text{sub.B}}T$ , where  $k_{\text{sub.B}}$  is the Boltzmann constant and  $T$  is the absolute temperature.

### Screening 1

[0158] Screening 1 focused on identification of materials of the first getter material that react with  $\text{CrO.sub.2(OH).sub.2}$  (80% rel. to  $\text{SrCO.sub.3}$ ) and do not react with  $\text{SO.sub.2}$  (150% rel. to  $\text{SrCO.sub.3}$ ). Additional considerations included the following conditions: reactivity with  $\text{NO.sub.x}$ ,  $\text{H.sub.2O}$ , temperature, cost, and no chlorides or fluorides.

[0159] The screening criteria generated **1037** materials shown in a scatterplot of FIG. 6A. The scatterplot summarized results by reactivity with  $\text{SO.sub.2}$ , reactivity with  $\text{CrO.sub.2(OH).sub.2}$ , and cost of the material. The more suitable candidates are located in the bottom right corner of the scatterplot.

[0160] A decision tree analysis was applied to filter out additional materials. The decision tree was trained on the overall reactivity metric. FIG. 6B shows the decision tree as learned. Darker squares indicate more preferred reactions and less undesired reactions. The figure of merit (“value”) is the  $R_{\text{sub.Cr}}-0.5*Rs$ , where a higher number (darker box) is more desirable.

### Screening 2

[0161] Screening 2 focused on identification of materials with chromium that are unlikely to react with  $\text{SO.sub.2}$  (110% rel. to  $\text{SrCO.sub.3}$ ). Additional considerations included the following conditions: reactivity with  $\text{NO.sub.x}$ ,  $\text{H.sub.2O}$ , temperature, cost, and no chlorides or fluorides.

[0162] The screening criteria generated 117 materials shown in a scatterplot of FIG. 7A. The scatterplot summarized results by reactivity with  $\text{SO.sub.2}$ , reactivity with  $\text{H.sub.2O}$ , and cost of the material. The more suitable candidates are located in the bottom left corner of the scatterplot. Materials including S, P, or both were identified as desirable.

[0163] A decision tree analysis was applied to filter out additional materials. The decision tree was trained on the overall reactivity metric. FIGS. 7B and 7C show the decision tree as learned.

[0164] Darker squares indicate more preferred reactions and less undesired reactions. The figure of merit (“value”) is  $-1*Rs$ , where a higher number (darker box) is more desirable.

### Screening 3

[0165] Screening 3 focused on identification of possible new materials that are likely to react with  $\text{SO.sub.2}$  (200% rel. to  $\text{SrCO.sub.3}$ ) and have a relatively low cost.

[0166] The screening criteria generated 925 materials shown in a scatterplot of FIG. 8A. The scatterplot summarized results by reactivity with  $\text{SO.sub.2}$ , reactivity with  $\text{CrO.sub.2(OH).sub.2}$ , and cost of the material. The more suitable candidates are located in the top portion of the scatterplot. Alkali earth metals were identified as desirable.

[0167] A decision tree analysis was applied to filter out additional materials. The decision tree was trained on the overall reactivity metric. FIGS. 8B and 8C show the decision tree as learned. Darker

squares indicate more preferred reactions and less undesired reactions. The figure of merit (“value”) is R.sub.S, where a higher number (darker box) is more desirable.

[0168] The analysis further studied the Gibbs free energy of formation of various reactions consuming SO.sub.3. Excess sulfur, if present in the component, is presumed to preferentially interact with the compositions as shown in the plot of FIG. 9. As can be seen from the plot of FIG. 9, the probability of the reactions of S with various materials listed below is in the following order of thermodynamic preference: [0169] (1) CaCO.sub.3—assuming it is not already chromated, highly likely to form a sulfate, CaCO.sub.3.fwdarw.CaSO.sub.4; [0170] (2) MgO—thermodynamically unlikely to form a carbonate, unlike other alkali earth oxides, MgO.fwdarw.MgSO.sub.4; [0171] (3) BaCrO.sub.4—may be used as a sacrificial material, reaction BaCrO.sub.4.fwdarw.BaSO.sub.4; [0172] (4) Other alkali earth chromates, CaCrO.sub.4.fwdarw.CaSO.sub.4, SrCrO.sub.4.fwdarw.SrSO.sub.4; [0173] (5) Chromia and alumina, Cr.sub.2O.sub.3.fwdarw.Cr.sub.2(SO.sub.4).sub.3, Al.sub.2O.sub.3.fwdarw.Al.sub.2(SO.sub.4).sub.3.

[0174] The processes, methods, or algorithms disclosed herein may be deliverable to or implemented by a processing device, controller, or computer, which may include any existing programmable electronic control unit or dedicated electronic control unit. Similarly, the processes, methods, or algorithms may be stored as data and instructions executable by a controller or computer in many forms including, but not limited to, information permanently stored on non-writable storage media such as ROM devices and information alterably stored on writable storage media such as floppy disks, magnetic tapes, CDs, RAM devices, and other magnetic and optical media. The processes, methods, or algorithms may also be implemented in a software executable object. Alternatively, the processes, methods, or algorithms may be embodied in whole or in part using suitable hardware components, such as Application Specific Integrated Circuits (ASICs), Field-Programmable Gate Arrays (FPGAs), state machines, controllers or other hardware components or devices, or a combination of hardware, software and firmware components.

[0175] While exemplary embodiments are described above, it is not intended that these embodiments describe all possible forms encompassed by the claims. The words used in the specification are words of description rather than limitation, and it is understood that various changes can be made without departing from the spirit and scope of the disclosure. As previously described, the features of various embodiments can be combined to form further embodiments of the disclosure that may not be explicitly described or illustrated. While various embodiments could have been described as providing advantages or being preferred over other embodiments or prior art implementations with respect to one or more desired characteristics, those of ordinary skill in the art recognize that one or more features or characteristics can be compromised to achieve desired overall system attributes, which depend on the specific application and implementation. These attributes can include, but are not limited to cost, strength, durability, life cycle cost, marketability, appearance, packaging, size, serviceability, weight, manufacturability, ease of assembly, etc. As such, to the extent any embodiments are described as less desirable than other embodiments or prior art implementations with respect to one or more characteristics, these embodiments are not outside the scope of the disclosure and can be desirable for particular applications.

## Claims

1. A method of reducing release of chromium from an electrochemical system, the method comprising: binding chromium-containing molecules from an airstream to a chromium getter material of an electrochemical system component while operating the electrochemical system to obtain bound chromium-containing molecules, the chromium getter material including a saturated state and an unsaturated state through at least a portion of a thickness of the chromium getter material; and treating the chromium getter material in the saturated state to reduce contact of the

bound chromium-containing molecules in the chromium getter material with the airstream.

**2.** The method of claim 1, wherein the chromium getter material in the saturated state has a surface portion and a bulk portion and wherein the treating includes diffusing at least a portion of the bound chromium-containing molecules from the surface portion to the bulk portion by increasing a temperature of the chromium getter material in the saturated state above an operating temperature and lowering a relative humidity and an oxygen partial pressure below a relative humidity operating value and an oxygen partial pressure operating value, respectively.

**3.** The method of claim 2, further comprising lowering the temperature of the chromium getter material, increasing the relative humidity, and increasing the oxygen partial pressure to the operating temperature, the relative humidity operating value, and the oxygen partial pressure operating value, respectively, when a predetermined unsaturated concentration is reached.

**4.** The method of claim 1, wherein the chromium getter material has a surface portion and a bulk portion and wherein the treating includes applying an amount of an overlay material adjacent the surface portion.

**5.** The method of claim 4, wherein the amount of the overlay material has a same chemical composition as the chromium getter material of the surface portion.

**6.** The method of claim 4, wherein the overlay material is a non-chromium getter material.

**7.** The method of claim 6, wherein the non-chromium getter material includes a chromium-free material.

**8.** The method of claim 1, wherein the electrochemical system component is an oxygen outlet component.

**9.** An electrochemical system component of an electrochemical system, comprising: a structural ceramic or metal portion; and a chromium getter material including an unsaturated surface layer; an unsaturated bulk portion; and a saturated middle layer disposed between the unsaturated surface layer and the unsaturated bulk portion, the saturated middle layer being free of a contact with an airflow in the electrochemical system component.

**10.** The electrochemical system component of claim 9, wherein the electrochemical system is an electrolyzer.

**11.** The electrochemical system component of claim 9, wherein the electrochemical system component is an oxygen outlet component.

**12.** The electrochemical system component of claim 9, further comprising a sulfur getter material separate from the chromium getter material.

**13.** The electrochemical system component of claim 9, wherein the unsaturated surface layer has a same chemical composition as the unsaturated bulk portion.

**14.** An electrochemical chromium monitoring system comprising: a controller programmed to monitor a concentration of chromium in a first chromium getter material portion of a first piping component of the electrochemical chromium monitoring system; redirect an airflow to a second piping component having a second chromium getter material portion when a predetermined saturation level of the first chromium getter material portion is detected, calculated, or projected; and transmit signals to treat the saturated first chromium getter material portion to achieve a predetermined unsaturated concentration of the first chromium getter material portion.

**15.** The system of claim 14, wherein the saturated first chromium getter material has a surface portion and a bulk portion and wherein the treating includes diffusing at least a portion of the bound chromium-containing molecules from the surface portion to the bulk portion by increasing a temperature of the first saturated chromium getter material above an operating temperature and lowering a relative humidity and an oxygen partial pressure below a relative humidity operating value and an oxygen partial pressure operating value, respectively.

**16.** The system of claim 14, wherein the second chromium getter material portion has a lower concentration of chromium than the first chromium getter material.

**17.** The system of claim 14, wherein the treating includes applying an additional amount of an

unsaturated chromium getter material over the first chromium getter material portion.

**18.** The system of claim 17, wherein the additional amount of the unsaturated chromium getter material has a same chemical composition as the first chromium getter material portion.

**19.** The system of claim 14, wherein the treating includes applying a layer of a non-chromium getter material onto the first chromium getter material portion.

**20.** The system of claim 14, wherein the electrochemical chromium monitoring system is an electrolyzer.

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