Several Aspects on Materials Problems for SCWR

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Abstract. The supercritical-water-cooled reactor (SCWR) system is being evaluated as a Generation IV concept because it builds on currently proven light water technology to provide for high thermal efficiency and plant simplification. Materials selection is a critical gap that development and a long term safety operation of the supercritical-water-cooled reactor (SCWR) need to be faced with. Design concept of increased temperature and pressure, radiation and supercritical water coolant brings into a more aggressive environment to candidate materials. ASME rules provide fundamental needs with various aspects as a guideline on nuclear power plant (NPP) design. This paper covers materials design requirements in ASME code section III subsection NH for elevated temperature components in NPP from the point of view at engineering design angle. Establishment of new codes and standards is needed for the deployment of materials in SCWR in use. Multidisciplinary cross research and application of advanced computerical material science in screening suitable materials and building in predicable performance in plant operating experience are recounted and proposed. In addition, the present situation and existing problems on industry production of candidate materials in China are introduced.

FORWORD

With the announcement of DOE, the supercritical water cooled reactor is being well known as one of six Generation IV nuclear reactor concepts. The supercritical water cooled reactor concept has obviously distinguishable areas from the traditional water-cooled reactor, which build on currently proven light water reactor technology and supercritical fossil plant technology to provide for high thermal efficiency and plant simplification. The main features of SCWR opinion^[1] (Yao et al.2006)are: Firstly, "coolant" is supercritical water that will be operated at above the critical point of water(374 °C/22.1MPa); the thermal efficiency can be increased more than that of present light water reactor because "supercritical water coolant" has typical characteristics of both liquid and gas. Secondly, SCWR is operated in the environment of high temperature, high pressure and high irradiation, which design pressure is about 25Mpa and reactor core outlet temperature is $510 \sim 550$ °C. The last, the heat-transfer style is simplified so that the pressurizer, the steam generator and the recycle pump, etc. in conventional light water reactor will be called off in SCWR. The main design parameters of SCWR are described in Table 1 below(Allen,2004). Figure 1 is the simplified configuration of SCWR. Even though many advantages of SCWR, these characteristics of increased temperature and pressure, radiation and supercritical water coolant brings into a more aggressive environment to candidate materials and multidiscipline interaction is also addressed for SCWR, such as material properties, water chemical and thermal-hydradulics, and etc. The need to develop materials capable of performing in the severe operating environments expected in SCWR reactors represents a significant challenge in materials science because of the significant challenges associated with structural materials in this advanced nuclear energy systems. The primary method currently envisioned to provide high strength.

99 99	Table 1 main parameters	
Supervices Water	Parameter	Value
	Thermal power	3575MWth
	Net electric	1600MWe
	power	
Fig. 1. SCWR concept	Net thermal	44.8%
	efficiency	
	operating	25MPa
	pressure	
	Reactor inlet	280℃
	temperature	
	Reactor outlet	510~550°C
	temperature	
	Irradiation dose	15~67dpa
	Reactor flow	1843kg/s
	rate	

and fracture toughness as well as appropriate radiation resistance for high-temperature metallic components. The objective of this paper is to covers materials design requirements in ASME code section III subsection NH for elevated temperature components in NPP from the point of view at engineering design angle and to recount advanced computer material science in screening suitable materials and building in predicable performance in plant operating experience. In addition, establishment of new codes and standards and multidisciplinary cross research for SCWR development are proposed.

2. REQUIREMENTS IN ASME CODE SECTION III NH SUBSECTION ^[2]

2.1. Selected Materials Described in NH subsection

ASME code Section III subsection NH applies to Class 1 components serving as pressure boundaries at elevated temperatures in nuclear power plant. The recommended materials used under elevated temperatures are 304 S.S. 316S.S.,21/4Cr-1Mo,9Cr-1Mo-1V and 800H alloy, as following table 2, given corresponding maximum service temperature.

Table 2 materials described in NH subsection

Materials	304SS	316SS	800H	2 1/4Cr-1Mo	9Cr-1Mo-1V
Max.temp.	800°C	800℃	800℃	650°C	650℃

2.2. Consideration with time-dependent materials property

Materials mechanical properties at elevated temperature are extremely sensitive to temperature. The behavior of materials at elevated temperatures mainly puts up time-dependent properties. Consideration with time-dependent properties for materials serving above a specific elevated temperature is taken in NH subsection. Creep is one typical time-dependent material property, that is, the special case of inelasticity that relates to the stress-induced time-dependent deformation under load. NH subsection pays attention to creep for Class 1 components engineering analysis as well as an expected loading history which consists of how each design parameter varies as a function of time because materials have time-dependence characteristic under higher temperature service is needed for design analysis. In NH subsection, creep-ratcheting phenomena resulted from creep is introduced. At least two mechanisms that high temperature engineering design must take into account are involved in creep ratcheting for materials: First, creep can alter the residual stresses and thus affect the time-independent behavior. Secondly, the time-dependent deformation can be enhanced because of the nonlinear interaction of primary and secondary stresses. Where creep effects are presumed significant, inelastic analysis is generally required to provide a quantitative assessment of deformation and strains so that Appendix T may be called for.

2.3. Inclusion of elastic analysis and inelastic analysis for design by analysis

Design by analysis includes elastic analysis and inelastic analysis as table 3. In NH subsection, the analysis for load controlled stress limits is elastic analysis while the analysis of strain, deformation and fatigue limits is inelastic analysis. Plastic and creep are special cases of inelasticity. When thermal and mechanical loadings are sufficiently severe to produce yielding and/or when thermal creep processes are active, inelastic design analysis may be required. This requires analysis of combined time-independent elastic-plastic material behavior and time-dependent creep behavior capable of predicting stresses, strains and deformations as functions of time for specific thermal-mechanical load histories.

Category	Features	Requirements
Elastic analysis	No significant creep	maximum shear theory \rightarrow
	effects.	stress intensities for multiaxial stress
		states.
Inelastic	Significant creep effects	Multiaxial stress-strain relationships
analysis		+ associated flow rules \rightarrow
		combine multiaxial stresses and strains.

Table 3 Design by Analysis

2.4. Structural integrity for class 1 components at elevated temperatures

Materials damage for structure integrity at elevated temperature includes fatigue damage, creep damage and creep-fatigue coupling effect in NH subsection as figure 2.Fatigue damage is that part of the total material damage caused by cyclic deformation which is independent of time effects(e.g., stress holdtime, strain holdtime, frequency). Creep damage is that part of the total material damage caused by time exposure to steady and transient stresses at elevated temperatures, expressed as a time ratio. Creep-fatigue interaction is the effect of combined creep and fatigue on the total creep-fatigue damage accumulated at failure. The effective and reasonable constitutive equations shall be established at first to use for describing the inelastic behavior for structure integrity analysis. The constitutive equations should reflect the following features when they have a significant influence on structure response: the effects of plastic strain hardening including cyclic loading effects and the hardening or softening which can occur with high temperature exposure; primary creep and the effects of creep strain hardening as well as softening (due to reverse loading); and the effects of prior creep on subsequent plasticity, and vice versa. Appendix T supplies the elastic and simplified inelastic methods of analysis to be used to establish conservative bounds for deformations, strains, strain ranges and maximum stress. Inelastic strains criteria for structural integrity is as table 4. Evaluation methods for strain limits are elastic analysis and simplified inelastic analysis specified in Appendix T.

Table 4 Inelastic strains criteria for structural integrity:

		0 9		
Maximum accumulated	Strains	averaged	strains at	local strains at
inelastic strain	though	the	surface ⁽¹⁾	any point
	thickness			
Limits criteria	$\leq 1\%$;	\leq 2%	\leq 5%

Note: due to an equivalent linear distribution of strain through the thickness.

The creep –fatigue interaction are considered for components served at elevated temperature. The combination of various service loadings shall be evaluated for accumulated creep and fatigue damage, including hold time and strain rate effects. The creep and fatigue damage shall satisfy the following relation.

$$\sum_{J=1}^{P} \left(\frac{n}{Nd}\right) j + \sum_{k=1}^{q} \left(\frac{\Delta t}{Td}\right) k \le D \quad , \tag{1}$$

 $\sum_{J=1}^{P} (\frac{n}{Nd})_{j}$ is for creep damage used by inelastic analysis; $\sum_{k=1}^{q} (\frac{\Delta t}{Td})$ is for fatigue damage used

by inelastic analysis; D shall not exceed the creep-fatigue damage envelope.

The appropriate design fatigue strain curve is used for evaluating fatigue damage. The creep damage is evaluated using the procedure of T-1433.

2.5. Example of 9Cr-1Mo-1V material

The candidate materials for SCWR comprise austenitic stainless steel, martensite-ferritic steel and nickel-base alloy while 9 Cr steels are one of



Fig. 2. Structural Integrity

recommended candidate materials. As described in table 2, 9Cr-1Mo-1V is defined in NH-subsection, which is specially mentioned.9Cr-1Mo-V has several unique characteristics accounted for below that material design and structure analysis for high temperature components shall be greatly given notice to:

- (a) There is not a clear distinction between time-independent elastic-plastic behavior and time-dependent creep behavior.
- (b) Flow stresses are strongly strain-rate sensitive at elevated temperature.
- (c) The material exhibits cyclic softening over the entire elevated-temperature use range and significant flow softening at 540° C and above.

However, NH subsection indicates, because decoupling of plastic and creep strains in the classical constitutive framework is generally a poor representation of the true material behavior for 9Cr-1Mo-1V, a plastic analysis for 9Cr -1Mo-1V shall generally account for rate dependence and creep effects. In addition, time-independent plasticity at higher temperatures occurs only in limiting cases for 9Cr -1Mo-1V steels where strain rates are high relative to creep rates.

The creep-fatigue coupling effects analysis for structure integrity for 9Cr-1Mo-1V shall follow the equation (1) accounted for above. Especially for 9Cr-1Mo-1V, the design fatigue curve at elevated temperature is as following figure 3 and the creep-fatigue damage envelop is in figure 4. The results of design by analysis and

structure integrity analysis for 9Cr-1Mo-1V materials for SCWR shall primarily meet the requirements in NH subsection.

3. ADVANCED COMPUTATIONAL MATERIAL SCIENCE IN RESEARCH ON SCWR

3.1. Significance of advanced computational material science for SCWR

The rising computational material science in recent decades manifests more and more predominant uniquely in the broad area of materials design, screening and research. Obviously, computational material science extends and supplements the traditional material science and has a significant impact on the development of material science.

The computational material science has made the great progress in developing and



Fig. 3. Design fatigue strain range

Fig. 4. Fatigue-creep damage envelop

researching advance reactor systems (ORNL,2004), especially in materials irradiation performance. The writer thinks the advanced computational material science can be taken as an effective assistant tool for solving related materials problems for development of SCWR and for future engineering application. An aggressive theory and modeling effort in computational material science will not only reduce the time but also experimental investment for research on the candidate materials for SCWR and that the quantity of design data can be also reduced in virtue of model predictions by computational material science for candidate materials in severe conditions in SCWR. Appropriate computational models can also take full advantage of data gotten from experiments for SCWR. The primary objective of computational material science is to develop predictive property models that account for the highly synergistic combinations of the candidate materials and environmental variables under SCWR conditions. Another objective of computational material science is to interpret materials property changes in engineering assessment of structure integrity in practical service conditions in NPP. The latter is very useful in engineering design. For SCWR, development of modeling and simulations of irradiation-induced materials property changes behavior in SCWR environment is firstly focus on. However, even though the potential for computational materials science is proved useful in designing materials and predicting materials' performance, the current research of the science is still crosscutting for SCWR.

3.2. Configuration on advanced computational material science

Theory and modeling in computational material science are helpful to be used as resultful description of materials phenomena and mechanism and assistant for structure analysis together with alloy design. But for those, computer experiments can not be left from. In addition, the fully and profound understanding of microstructure evolution and activities of

defects in alloy must be the basis on building on the theory and modeling and simulation. Further, models of microstructure evolution and defects activities form fundamentals of description and understanding of many materials properties varying with aggressive environment conditions in NPP. Rapid progress of computer science is a second conditioned factor for computational material science. Currently numerous software and analysis tools as well as good hardware environment also drive the rise and grown up of computational material science. Mathematics knowledge is useful measure for computational material science. It is very helpful to establish, develop and apply theory and models using mathematics tools. Finally, modeling efforts must be linked to a wide variety of experiments to understand mechanisms, measure key parameters, and validate and calibrate model predictions. Codes, standards, regulations are also used for verification and validation of reasonableness of models and simulations prediction. Figure 5 shows configuration of each concept relevant to advanced computational material science.

3.3. Problems needed to solve for SCWR by advanced computational material science^[3]

Those environment variables of SCWR are different from traditional light water reactor make computational material science be in face of challenges at setting up models of many materials properties. For one characteristic of coolant inlet temperature/outlet temperature 280/510°C,transient near 800°C for SCWR, the material issues needed to model and assess the capability at higher temperatures and across a wide temperature range include: thermal creep, fatigue /thermal fatigue,



Fig. 5. Configuration on advanced computational material science

creep-fatigue interaction, toughness, corrosion /SCC and thermal- hydradulics effects. For another characteristic of high fluence /dose for SCWR because irradiation dose is 15 dpa for removable components and irradiation dose is close to 67dpa for core barrel, the question is modeling needed to set up toward a prediction of following material properties in candidate materials under high irradiation exposure: void swelling, irradiation creep, creep crack growth, creep rupture and stress relaxation, embrittlement and irradiation accelerating stress corrosion cracking. For the third main characteristic of unique chemical environment of supercritical water above water "critical point" for SCWR, the major problems needed to solve for computational material science are modeling to predict the candidate materials property behaviors under chemical interaction subject to large radiation dose, such as corrosion, oxidation, compatibility, IASCC, EAC, and coupling combination effects of chemical parameters and irradiation, etc..

In these studies, the co-evolution of the microstructure of components, and their roles in the macroscopic response in terms of swelling, irradiation creep, and radiation -induced phase transformations must be emphasized on within the SCWR development, (Alen,2004).

3.4. Major progress of computational materials science for nuclear application ^[4]

Computational material science has been used to build on modeling and prediction of elevated temperature properties and irradiation properties in nuclear application. A typical example is development of physically-based models of reactor pressure vessel irradiation-induced embrittlement and other irradiation damage effects including void swelling in traditional light water reactor (LWR). The writer believes that the successful experiences from modeling LWR components will extend to apply for SCWR analysis, while a perfect model must be closely description of the researched materials performance and prediction of the materials properties even degradation trend under environment variables (temperature, dose, dose rate, stress, etc.) accounted for in life time by well interpolating or extrapolating method, etc. Currently, because the microstructure investigation research indicates (ORNL,2004) elevated temperature and irradiation dose in nuclear reactor change defects activities in the materials with complex mechanism, microstructure evaluation such as defects activities, segregation, etc. must be source on establishing modeling and simulations prediction of irradiation properties changes of irradiated materials, which models of void swelling has linked voids effects and network dislocations activities. Now 3-dimensional dislocation dynamics involving in dislocation climb models are encouraged to quantitatively apply to investigations of microstructural evolution of irradiated materials. It is reported (ORNL, 2004) a further challenge is how to develop the appropriate linkages of 3-dimensional dislocation dynamics to atomic scale and mesoscale regimes so that multiscale phenomena such as fracture toughness can be appropriately modeled.

While many models have been opened out, the ability to integrate modeling components is still lacking. But a more extensive behavior of theory and modeling could make significant progress in dealing with critical issues related to structural materials application in Gen-Iv.

4. DEVELOPMENT OF NEW CODES AND MULTIDISCIPLINARY CROSS RESEARCH

4.1. Necessity on development of new codes for SCWR

Codes, regulations and standards are important assurance for reactor function; safety and operation while also are one of important verification techniques for reactor system design. In the other hand, Codes, regulations and standards that can successfully predict experimental results before the experiments are performed provide the most reliable predictions on engineering applications. During development of advanced nuclear reactor system, ASME code NH subsection for class 1 components at elevated temperatures does not fully consider with other environment variables except temperature, stress, time and SCWR is also a new concept for nuclear components suppliers (responsible for nuclear components design and manufacture). In addition, SCWR has larger output power, higher coolant temperature and pressure and stronger radiation exposure than those of conventional light water reactor (LWR), that must be considered for options and design of materials. Because brand-new concept of reactor system and aggressive environment conditions and advanced materials development, new codes, regulations and standards are urgently needed to be brewed, drawn up and developed for engineering design along with gradual progress of innovation of SCWR techniques and for licensing by USNRC. For computational material science, new codes also are a problem for engineering utility. For engineering purpose, the computed and measured property changes by computational material science need to be codified into approbatory information by related codes, which an engineer can use to design a nuclear energy system, assess its performance, and determine its ultimate lifetime. Validation and verification of the predictions made by computational models also are needed by using either established benchmarked computational codes or experimental data. The demands for new codes, regulations and standards are driven by ultimate engineering purpose.

4.2. Necessity on development of multidisciplinary cross research

The thermal-hydradulics (fluid field and temperature field) in reactor core of SCWR has been closely coupling relationship with behaviors of various reactor materials. The main differences of reactor core between SCWR and conventional light water reactor(PWR and BWR) are coolant temperature (from 280°C~510°C),that is boundary conditions are different; in addition, the major physic parameters of "the supercritical water", such as specific heat and "water" density, etc. will abnormally change at about "critical point" to result in creating influence on structure stability of class 1 components. In the other hand, it is also a problem needed to probe into that coupling relationship between water chemistry of coolant in SCWR and anti-corrosion properties of candidate materials. These shows that materials research performed simply and singly may not represent the real behaviors of candidate materials under a rigorous environment in SCWR. Therefore, multidisciplinary cross research is called out in screening materials and evaluating materials properties during the development of SCWR.

5. CURRENT SITUATIONS IN CHINA OF THE CANDIDATE MATERIALS PRODUCTION

Here describes materials production of (ultra)supercritical fossil power units in China. With the introduction and development of techniques of (ultra)supercritical foil power units, China

began to develop and manufacture steels serving with elevated temperature properties by ourselves, including pipes, forgings and casting. Evaluated steels^[5](hu, 2005)involve in: steels for boiler tubes (12Cr1MoV, T91 (SA-312), TP304H, TP347H); big bore seamless pipes (P22, P91, 12Cr1MoV); and steels for vanes of turbines for subcritical units (17-4PH, AISI405) and thick plates, etc.. But some key boiler materials still depends on import from foreign countries. In many cases, design techniques have been mastered by our country but manufacture industries exit a big gap from famous enterprises in the world, which one problem is materials manufacture, such as heavy section forgings. Acceleratory development of materials production industry is an urgent problem currently faced by the field of industries in China.

6. CONCLUSIONS

(1)SCWR concept is set up on the basis of currently proven technology of light water reactor and supercritical foil plant with supercritical water coolant, high thermal efficiency and plant simplification.

(2)ASME code NH subsection applies to class 1 components serving as pressure boundaries at elevated temperatures in NPP and considers with time-dependent materials properties for design by analysis which includes elastic analysis and inelastic analysis. Structure integrity for class 1 components at elevated temperature in NPP is focus on in NH subsection which accounts for fatigue damage, creep damage and fatigue-creep interaction needed to meet the strain limits.9Cr steels are recommended for SCWR concept design, which 9Cr-1Mo-1V steels is specially mentioned and needed to take notice on because they have unique characteristics influence on design by analysis.

(3)Advanced computational materials science has great impact on material screening, material development and material research to helpfully apply to design of advanced reactor system and has made quite progress in irradiated materials, which link microstructure evolution and materials performance under environment variables. Materials problems needed to solve by computational material science in future for SCWR include embrittlement, creep, swelling, irradiation creep, fatigue and corrosion, IASCC etc. under materials subject to severe environment variables.

(4)New codes, standards and regulations needed to develop because they are safety assurance of engineering application of SWCP construction and also are verification and validation technique for research and experiments for future design for SCWR. In addition, necessity of multidisciplinary cross research is required in whole research works for SCWR.

(5)In China, manufacture capacity of candidate materials for SCWR is needed to strengthen and acceleratory development of materials production industry is an urgent problem currently faced by the field of industries in China.

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