

## Research on Mechanics and Mechanisms of Stress Corrosion Cracking Based upon Mechano-Chemical Oxidation Kinetics

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### 【Outline of survey】

Aiming at fundamental and essential mitigation of the stress corrosion cracking (SCC) of the structural materials in light water reactor (LWR) environments, a new material design concept, i.e., the development of guideline for the 3rd generation austenitic stainless steels and nickel base alloys will be constructed on the basis of SCC propagation mechanism. The propagation of SCC is thermodynamically consequential in these materials and control of crack growth rate is an engineering target. Especially, through interdisciplinary cooperation among the researchers with various backgrounds such as mechanical engineering, chemistry and physics, it is possible to effectively promote the next-generation material development based on the essential mechanism of the SCC propagation which is the most important materials degradation mode in nuclear power plants.

We focus the effort to the oxidation phenomenon accompanied with mass transport in the singular stress field at the crack tip region (crack oxidation model) which has been proposed and clarified by this group, who has been pioneering mechanism research world widely. The oxide formation energy and the oxygen diffusion kinetics will be evaluated quantitatively by quantum chemistry molecular dynamics and stress acceleration diffusion calculation. Aiming at the construction of the development base of austenitic alloys that is highly resistant to SCC, a quantitative evaluation of these characteristics and a research on the effects of various additional alloying elements both in the iron base alloys and in the nickel base alloys will be performed. The materials proposed for exploration of the best performance for SCC, will be tested in simulated LWR environments and be analyzed based on the unique theoretical formulation proposed by the group. In order to verify this approach more fundamentally, cooperation with Professor Ahmed Zewail (California Institute of Technology, the Nobel winner in chemistry, 1999), has started for verification of the molecular dynamics in atomic level.

### 【Expected results】

The research group had conducted the Center of Excellence Program on "Physics and Chemistry of Fracture" with a special support by the Ministry of Education, Culture, Sports, Science and Technology (MEXT), Japan for five years (1999-2003). The major part of the outcome of the program is a basis of this program and has been world widely accepted and cited in many publications including ASM Handbook. In the program, the theoretical formulation of crack growth rate, in which the synergy of the crack tip mechanics based on the continuum mechanics approaches and the oxidation kinetics at crack tip region, was focused and a new academic area of Physics and Chemistry of Fracture was proposed. Consequently, as one of the important issues in the cracking, an importance of the quantitative evaluation of stress accelerated oxidation kinetics was pointed out and precursory introduced to the research area.

In this research program, development guideline for the 3rd generation alloys with an excellent performance for SCC, so called SCC-free alloys will be proposed based upon a fundamental and essential mechanism of SCC propagation. Namely, on the basis of SCC propagation mechanism where the quantum chemistry molecular dynamics and reaction dynamics is taken into account, the prototype 3rd generation alloys will be fabricated. The methodology of material development for the alloys which could be one of the essential solutions of SCC problem both in aged and in next-generation LWRs will be proposed.

### 【References by the principal researcher】

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- 2). Tetsuo Shoji, "Progress in the mechanistic Understanding of BWR SCC and Its Implication to the Prediction and SCC Growth Behavior in Plants" Proceedings of 11th International Conference on Environmental Degradation of Mechanicals in Nuclear Power Systems-Water Reactors. August 10-14, 2003, Stevenson, Washington, ANS Paper, No81906

【Term of project】 FY 2005 - 2009

【Budget allocation】 85,900,000 yen

【Homepage address】 <http://www.rift.mech.tohoku.ac.jp/index.html>