CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES

TRIP REPORT

SUBJECT: Attendance to the 203rd Meeting of the Electrochemical Society
Charge Number: 20.06002.081; AI 06002.01.081.311

DATE/PLACE: April 28—May 2, 2003; Paris, France

AUTHOR: Osvaldo Pensado

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PERSONS PRESENT:

The conference attracted 2,997 papers presented in 57 technical symposia. This meeting has been the most attended in the history of the Electrochemical Society, with participants from academia, research institutions, and industries from all over the world, interested in electrochemical and solid state technology. The complete list of authors is available in the meeting abstracts volume published by the Electrochemical Society. Any interested person may request to borrow a copy of the meeting abstracts volume from the author.

BACKGROUND AND PURPOSE OF TRIP:

The Electrochemical Society is an international, nonprofit, educational organization concerned with a broad range of phenomena relating to electrochemical and solid state science and technology. Two or three conferences organized by the Society are held every year. This year, the conference included symposia such as Passivity and Surface Structures for Corrosion Protection constituting a unique forum attracting worldwide experts in metal passivity. The author presented a paper based on a Center for Nuclear Waste Regulatory Analyses (CNWRA) study of passivity of proposed high-level waste container materials in the U.S. and gather criticisms and feedback from experts. Another objective for attending the meeting was to learn the latest developments in electrochemical science and technology, new approaches to study metals, and be informed of work sponsored by the U.S. Department of Energy (DOE) on corrosion of Alloy 22.

SUMMARY OF PERTINENT POINTS:

The author presented a paper titled A Mechanistic Model for the Passive Dissolution of Ni-Cr-Mo Alloys in the symposium Passivity and Surface Structures for Corrosion Protection. Feedback was gathered from experts in the field of passivity. It is recommended to submit a journal article to the Electrochemical Society summarizing our understanding of passive dissolution of Alloy 22.

Papers sponsored by the DOE on corrosion of Alloy 22 were canceled.

Papers presented in the symposium Computational Chemistry covered fundamental Monte Carlo and molecular dynamics approaches to study electrochemical systems. Results are encouraging, but current capability for application to real systems is still limited.

SUMMARY OF ACTIVITIES:

Talks of interest are indicated:

The inaugural plenary talk was given by Gerd K. Binnig, winner of the 1986 Novel Prize in physics for the invention of the scanning tunneling microscope. Binnig is also inventor of the atomic force microscope. In the plenary talk, he concisely described the principles governing the atomic force and tunneling microscopes. Binning presented his proposal for a future memory device known as the millipede. Each leg of the millipede will be of atomic dimensions, capable of retrieving information stored in grids recorded in a substrate (similar to old music records). Deleting of the data will be accomplished by annealing the substrate.

The symposium on Passivity and Surface Structures for Corrosion Protection was organized by talks on elements, coatings, and inhibitors. R. Rapp delivered the paper Role of the Metal/Oxide Interface in the Growth of Passive Films in Aqueous Environments. He discussed work previously published in the field of high-temperature oxidation but not frequently referred to by aqueous-corrosion experts. He discussed that dissolution of metals via the transport of cations through the film necessarily results in the formation of vacancies in the alloy. Rapp stated that cation vacancies arriving at the metal/scale interface are annihilated by the climb of misfit and misorientation interfacial dislocations. If this mechanism is blocked, for example by the tangling of dislocations within the metal, then the growth of an adherent oxide cannot be guaranteed. O. Pensado presented the paper A Mechanistic Model for the Passive Dissolution of Ni-Cr-Mo Alloys. This work is consistent with Rapp's mechanism for the creation of vacancies in the alloy. We suggested that decays in time of the passive current density measured potentiostatically in Alloy 22 during 2-week periods are due to the accumulation of vacancies at the metal-film interface. As mentioned by Rapp, a dissolution process causing the accumulation of vacancies at the metal/film interface could produce a non-adherent oxide. However, we suggested that breakdown of passivity is not likely to be sustained for extended periods, given the excess of chromium with respect to nickel near the metal-film interface, indicated by the model computations, favoring the reformation of passivating chromium-rich oxides. Positive feedback on our work was gathered from experts such as P. Marcus, S. Fujimoto, and M. Bojinov. Therefore, it is recommended summarizing our work and submitting a paper to the Journal of the Electrochemical Society.

Other scheduled papers on Alloy 22 by G. Ilevbare (LLNL) and Digby D. Macdonald (Penn State University) were not presented.

A relatively high number of papers on *in situ* techniques to study corrosion processes were presented; for example, D. H. Kim discussed the use of X-ray reflectivity to track film thickness as a function of time and applied potential. X-ray reflectivity requires a synchroton to be implemented. P. Allongue used surface enhanced Raman spectroscopy to study *in situ* the formation and dissolution of passive layers in iron. Rather than activating the surface by the deposition of gold or silver nanopartcles on the oxide, Allongue proposed electrodepositing iron on gold substrates. The effect of aging on Fe-Ni alloys was studied by G. Lorang, et al. using Auger electron spectroscopy and X-ray photoelectron spectroscopy. Lorang argued that dissolution kinetics become slower as time elapses; therefore, aging results in more protective oxides. Interestingly, the more protective oxides are thinner. J. Noel discussed the use of *in-situ* neutron reflectometry as a non-destructive means to determine materials composition and layer thicknesses in the range 0.5–300 nm. For this technique the sample surface must be

smooth; also, the sample must be thin (hundreds of microns). Neutron reflectometry has been used mainly for the study of metallic elements at the University of Western Ontario.

P. Schmuki presented an interesting talk on the anodization of titanium and growth of highly ordered porous titanium oxide. Growth of the ordered structure requires of optimized electrolyte conditions containing hydrofluoric acid to activate the oxide. Under highly anodic potentials (~20 V), the metal grows a very thick oxide, up to 500 nm. Possibly these organized structures may have some application in nanotechnology. This paper offered additional insight on the activation of the oxide dissolution process by the presence of fluoride in the electrolyte.

Of special interest was the symposium on Computational Chemistry including presentations on state-of-the-art Monte Carlo and molecular dynamics simulations of electrochemical processes. Recent advances are promising; however, analyzed systems are simplified idealizations compared to real systems. For example, modeled systems comprise few molecules, with well defined orientations, interacting with perfect or near perfect crystals, and with simulations spanning a few nanoseconds. The modeling results allows us to understand or rationalize fundamental mechanisms of electrochemical processes; however, predictive capability on real systems of these fundamental models is still limited.

IMPRESSIONS/CONCLUSIONS:

Attendance to the conference supported the objective of keeping up to date in recent advances in electrochemical science and technology, and in the field of passivity. Participation in this prestigious international conference facilitated contact with international scientists. In general positive feedback was gathered on our work. We are current in our approach to study passive dissolution of Alloy 22.

PROBLEMS ENCOUNTERED:

None.

PENDING ACTIONS:

None.

RECOMMENDATIONS:

By disseminating CNWRA work among peers, we gather feedback for improvement. Attending the Electrochemical Society Meeting also allowed us to be better informed, and improve our skills in the use of electrochemical science and technology. Therefore, it is considered that attending this conference supports the Strategic Plan goals/strategies of (i) maintaining safety, protection of the environment, and the common defense and security, (ii) increasing public confidence, and (iii) making NRC activities and decisions more effective, efficient, and realistic. Consequently, it is recommended to continue attending to future Electrochemical Society meetings covering topics of interest to the NRC.

SIGNATURES:

Osvaldo Pensado
Senior Research Scientist

5/22/2003
Date

for V. Jain

Vijay Jain, Manager
Corrosion Science and Process Engineering

5/22/2003
Date

CONCURRENCE:

Budhi Sagar
Technical Director

5/22/2003
Date