Effect of non-random atomic arrangements on the initiation of passivation in solid-solution alloys

D. M. Artymowicz, K. Sieradzki and R.C. Newman

Department of Chemical Engineering and Applied Chemistry, University of Toronto

200 College Street, Toronto, ON, CANADA, M5S3E5

Passivation of solid-solution alloys must, at some level, be related to the arrangement of the metal atoms in three dimensions. For the case of a random solid solution, significant results have been obtained experimentally and by atomistic simulation, leading to hypotheses for important transitions such as the parting limit for de-alloying of a solid solution [1], or the 13% Cr criterion for passivation of stainless steel [2]. For engineering alloys, the unequal pairwise atomic interactions generate a non-random solid solution whose initial corrosion behaviour depends on the effective temperature at which the atomic arrangement is equilibrated. In-service ageing of such alloys will be important for the integrity of future energy systems. Conventional percolation criteria for connectivity of susceptible or protective atoms in 3D are altered compared with the random case.

Kinetic Monte Carlo simulations have shown that like-with-like clustering within the metal lattice can lower the passivation threshold significantly, while a tendency towards ordering raises the threshold. Experiments are in progress to test the relevance of such findings.

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2. K. Sieradzki and R.C. Newman, A percolation model for passivation in stainless steels. *J. Electrochem. Soc*., **133**, 1979-1980 (1986).