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MODELING OF SURFACE SEGREGATION OF Cr IN THE WCrY SMART ALLOY

Self-passivating Metal Alloys with Reduced Thermo-oxidation (SMART) are promising candidates for the first wall of the DEMOnstration power plant (DEMO). These materials aim at having an increased oxidation resistance during accidental conditions and acceptable plasma performance during regular operation of the power plant.

In this work, a tungsten-chromium-yttrium SMART alloy (WCrY) with a composition of 68 at% of W, 31 at% of Cr and 1 at% of Y is studied. Previous research already showed superior oxidation behavior in comparison to that of pure tungsten [1,2], and first experimental results were obtained for the material's behavior under plasma loading [1]. However, a detailed physical understanding of the interplay between sputtering, segregation and diffusion of the alloying elements inside the material during plasma exposure is still missing.

To obtain a better understanding of these processes and assess their effect on the surface concentrations, a phenomenological transport model based on the work of Ho [3] is proposed. Ho's model, which includes diffusion and sputter erosion only, is complemented by a segregation flux term to allow for diffusion against a concentration gradient of the alloying elements toward the surface.

Based on the experience that surface segregation affects the near surface region only, a three parameter segregation flux term is proposed. It includes a segregation constant K, a characteristic length L and the equilibrium surface concentration c_{eq}. The model is applied to annealing experiments at 800 K and 1000 K conducted by Koslowski et al. [4,5]. Good agreement between simulation and measured data is obtained using L = 2 nm, $K_{800K} = 4\cdot10^{-6}$ nm/s, $K_{1000K} = 4\cdot10^{-3}$ nm/s, and diffusion coefficients of Cr in the WCrY matrix of $D_{800K} = 1\cdot10^{-6}$ nm²/s and $D_{1000K} = 1\cdot10^{-3}$ nm²/s.

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