

MM 4: Topical Session Interface-Dominated Phenomena - Diffusion

Time: Monday 15:15–16:15

Location: H2

Invited Talk

MM 4.1 Mon 15:15 H2

Investigation of the early stage of reactive interdiffusion in the Cu-Al system by in-situ transmission electron microscopy — FLORENT MOISY¹, ●XAVIER SAUVAGE², and ERIC HUG¹ — ¹CRISMAT Ensicaen, Caen, France — ²GPM University Rouen Normandy, Rouen, France

The early stage of the reactive interdiffusion in the Al/Cu system was investigated by in-situ TEM at 350°C and 300°C. Original Al/Cu interfaces were created by a purely mechanical process using co-deformation at room temperature by drawing. During the reactive interdiffusion three IMCs were detected: Al₂Cu and AlCu grew in the Al side and the Al₄Cu₉ in the Cu side. Systematic comparisons with ex-situ annealed samples and with regions out of the electron beam proved that there was no significant artefact (thin foil or beam effect). Although GBs may act as fast diffusion path, no preferential growth of IMC along these defects could be observed. The mean growth rates of all IMCs follow a classical parabolic law indicating that the kinetic of the transformation is controlled by diffusion mechanisms. A strong deviation was observed however in the early stage of the reaction. Nanoscaled Mg₂Si particles located in the Al phase strongly interact with the transformation front. It leads to large fluctuations of the velocity of interphase boundaries at the nanoscale. The pinning effect in connection with change in local concentration gradients and driving forces will be discussed.

MM 4.2 Mon 15:45 H2

Silver-rich clusters reveal the initial ligament size during nanoporous gold dealloying via kinetic Monte Carlo simulation — ●YONG LI^{1,2}, JÜRGEN MARKMANN^{2,1}, and JÖRG WEISSMÜLLER^{1,2} — ¹Institute of Materials Physics and Technology, Hamburg University of Technology, Hamburg, Germany — ²Institute of Materials Research, Materials Mechanics, Helmholtz-Zentrum Hereon, Geesthacht, Germany

When nanoporous gold is made by dealloying Ag-Au, residual silver forms clusters that impact the material's functional properties. We point out that the clusters carry information on the geometry of the initial nanoscale network. Using atomistic kinetic Monte Carlo simulation, we studied the evolution of silver-rich clusters and ligament size for dealloying at various potentials. Our simulations demonstrate that dealloying involves two distinct stages. Primary dealloying generates the initial ligament network, while secondary dealloying brings coarsening of the ligaments and further dissolution. During primary

dealloying, the sizes of clusters and ligaments are constant over time and they decrease with increasing dealloying potential with a Gibbs-Thompson type relation. At this stage, the ratio between ligament size and clusters size is 1.30 ± 0.07 and independent of the potential. During secondary dealloying, the ligament size (L) for dealloying with various potentials converge to a common coarsening law, $L \propto t^{1/4}$. By contrast, the silver-clusters size still remains constant. That observation establishes that the surviving clusters provide a way to measure the initial ligament size.

MM 4.3 Mon 16:00 H2

Theoretical aspects of the reactive element effect — ANDY CHEN¹, ARTHUR HEUER¹, MATTHEW FOULKES², and ●MICHAEL FINNIS² — ¹CWRU, Cleveland OH, U.S.A — ²Imperial College London, UK

We are interested in the mechanism of growth of alumina scales on aluminium-containing alloys, and how the presence of certain elements such as Hf, Zr and Y operates to retard the growth of such scales, thereby improving their adherence and protective quality. These questions have been open for several decades, and are still not completely resolved [1]. We report here some recent results of experiments and theory, and in-sights that we have obtained. From tracer diffusion experiments, followed by Time of Flight - Secondary Ion Mass Spectroscopy (TOF-SIMS), diffusion coefficients of O and Al through alumina scales have been estimated and compared with measurements of weight-gain. Noting that grain boundaries are now believed to be the route for ion and electron diffusion, both of which are necessary for oxidation, we have applied Density Functional Theory to calculate the segregation energy of these reactive elements to a range of sites on grain boundaries in α -Al₂O₃, using our previous models of grain boundary structure [2]. Segregation of Hf and Zr and oxygen vacancies to the grain boundaries is favoured, with a spread of energies that we assess, and our calculations suggest how this may indirectly reduce the mobility of ions or electrons. Shortcomings of the classical theory of oxidation [3], originally due to Wagner, are discussed. The evidence is now overwhelming that the conventional hopping of cation and anion vacancies is not a relevant process.

[1] W. T. Chen, B. Gleeson, and A. Heuer. Oxidation of Metals, 92(3-4):137-150, 2019. [2] Hannes Guhl, Hak-Sung Lee, Paul Tangney, W. M. C. Foulkes, Arthur H. Heuer, Tsubasa Nakagawa, Yuichi Ikuhara, and Michael W. Finnis. Acta Materialia, 99:16-28, 2015. [3] A. Atkinson. Reviews of Modern Physics, 57:437-470, 1985.