

MM 40 Diffusion I

Zeit: Dienstag 10:30–11:30

Raum: TU H2038

MM 40.1 Di 10:30 TU H2038

Simulation of Internal Oxidation of Engineering Alloys under Industrial Process Conditions — ●JÜRGEN GEGNER — SKF GmbH, Material Physics, Ernst-Sachs-Str. 5, D-97424 Schweinfurt

Internal oxidation is of great technical importance as effective dispersion-hardening method or undesirable side effect to steel heat treatments. Reaction kinetics is usually described by Wagner's theory that is designed for laboratory conditions but does not sufficiently cover industrial operations due to the restriction to homogeneous concentration distributions of the less noble component M within the matrix metal, isobaric and isothermal processes. In order to overcome these limitations, a computer model based on iterative solution of Fick's law for the in-diffusion of oxygen with arbitrary initial distribution of M atoms is proposed. The solubility product and the stoichiometry factor of the precipitating oxide define the mass balance relationship. For homogeneously dissolved M atoms and isothermal-isobaric reaction conditions, it is shown that the results agree excellently with Wagner's theory and experimental data. Heterogeneous M distributions as well as nonisobaric and/or nonisothermal internal oxidation are accessorially covered by the new model. Illustrative processes are calculated and the results are discussed in detail.

MM 40.2 Di 10:45 TU H2038

Hyperfein Wechselwirkung von implantierten ^{111}Cd -Sonden im Hf_2Au Gitter — ●P. WODNIECKI^{1,2}, M. UHRMACHER², A. KULINSKA^{1,2}, B. WODNIECKA¹ und K.P. LIEB² — ¹IFJPAN, Krakow, Polen — ²II. Physikalisches Institut, Universität Göttingen

Wir berichten über PAC Messungen der elektrischen Feldgradienten, die man mit der Sonde $^{111}\text{In}/^{111}\text{Cd}$ im Hf_2Au Gitter findet. Dieses Gitter bildet sich in einer einfachen tetragonalen C11_b Struktur, deren Prototyp MoSi_2 ist. Es handelt sich dabei um die D_{4h}^{17} -Raumgruppe. Zwei Au-Atome und vier Hf-Atome bilden die Einheitszelle. Alle Plätze [Hf: 4(e)4mm, Au: 2(a) 4/mmm] sind achsialsymmetrisch bezgl. der c-Achse und der EFG Tensor ist diagonal an jedem Gitterplatz der Struktur.

Der Gitterplatz der implantierten In-Sonden ist in diesem Gitter unvorhersehbar, da man In als Verunreinigung in der Hf_2Au Matrix ansehen muss. Als weitere Unwägbarkeit könnte sich der eingenommene Gitterplatz der PAC-Sonden mit der Temperatur ändern. Diesen Fall haben wir bei der Untersuchung von TiPd_2 beobachtet, das in der gleichen Struktur vorliegt [1]. Daher war das Hauptanliegen der Untersuchung, die Hyperfein-Wechselwirkungsparameter in einem weiten Temperaturbereich zu messen, um die besetzten Gitterplätze und mögliche Platzwechsel zu beobachten.

[1] P. Wodniecki, B. Wodniecka, A. Kulinska, M. Uhrmacher, K.P. Lieb, *J. Alloys and Compounds* 385 (2004) 53.

MM 40.3 Di 11:00 TU H2038

Grain Boundary Radiotracer Diffusion and Segregation of Fe and Ni in Polycrystalline Cu — ●JENS RIBBE, SERGIY DIVINSKI, GUIDO SCHMITZ, and CHRISTIAN HERZIG — Institut für Materialphysik, Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany

^{59}Fe and ^{63}Ni grain boundary (GB) diffusion in high-purity Cu was measured by the radiotracer method combined with mechanical sectioning technique in an extended temperature interval. At higher temperatures the conditions of Harrison's *B* kinetics were satisfied and the triple product $P = s \cdot \delta \cdot D_{\text{gb}}$ of the segregation factor *s*, GB width δ , and the GB diffusivity D_{gb} was determined at selected temperatures. Performing GB diffusion measurements at lower temperatures under the *C* regime conditions, the GB diffusion coefficient D_{gb} was directly measured. Using the estimate of the GB width deduced from GB self-diffusion measurements on FCC metals, $\delta \approx 5 \cdot 10^{-10}$ m, the segregation factor *s* of Fe was determined as $s = P/\delta D_{\text{gb}}$. Fe reveals high segregation and very slow diffusivity D_{gb} in Cu high-angle GBs. However, the measured triple product P^{Fe} for Fe GB diffusion is by orders of magnitude larger than the GB diffusivity P^{Ni} of Ni. The main reason is the strong GB segregation of Fe in Cu.

MM 40.4 Di 11:15 TU H2038

Nickel Radiotracer Diffusion in B2 Ordered $\text{Ni}_{50-x}\text{Fe}_x\text{Al}_{50}$ Alloys — ●SERGIY DIVINSKI¹, FRANK HISKER¹, WOLFGANG LÖSER², ULF SÖDERVALL³, and CHRISTIAN HERZIG¹ — ¹Institut für Materialphysik, Universität Münster, Germany — ²IFW Dresden, Dresden, Germany — ³Department of Physics, Chalmers University of Technology, Göteborg, Sweden

Ni bulk diffusion was measured in a series of B2 ordered $\text{Ni}_{50-x}\text{Fe}_x\text{Al}_{50}$ alloys. The ^{63}Ni radioisotope in combination with the serial sectioning technique was applied at higher temperatures and the secondary ion mass spectrometry (the ^{64}Ni isotope) was used in a low temperature range. In the temperature interval from 1050 to 1500 K, well-type Arrhenius temperature dependencies were established for all studied compositions. As the Fe content *x* in the $\text{Ni}_{50-x}\text{Fe}_x\text{Al}_{50}$ ternary alloys increases, the Ni diffusivity generally increases. The activation enthalpy *Q* of Ni diffusion changes strongly non-monotonously in the ternary alloys between the binary end-members NiAl and FeAl revealing a pronounced minimum at the $\text{Ni}_{40}\text{Fe}_{10}\text{Al}_{50}$ composition and a conspicuous maximum around the $\text{Ni}_{25}\text{Fe}_{25}\text{Al}_{50}$ composition. The latter indicates additional ordering (e.g. of the L_{21} type) in the corresponding alloys.