MM 21 Intermetallische Phasen II

Zeit: Samstag 11:00–12:15 Raum: TU H2038

MM 21.1 Sa 11:00 TU H2038

Microstructural characterization of Inconel 706 alloy — •V. Kindrachuk[1], N. Wanderka[1], J. Banhart[1], D. Del. Genovese[2], and J. Rösler[2] — [1]Hahn-Meitner-Institut Berlin, Glienicker Str. 100, 14109 Berlin, Germany — [2]Technical University Braunschweig, D-38106 Braunschweig, Germany

Inconel 706 is a wrought Ni-Fe base superalloy which is used for applications at service temperatures up to 600°C. It develops its good mechanical properties by precipitation of intermetallic phases γ' ($L1_2$ structure) and γ" (DO_{22} structure) in the austenitic γ matrix. Microstructure evolution was studied after ageing times of 750 h and 5000 h at 750°C. Characterization of the precipitates and of the matrix was carried out by three-dimensional atom probe tomography and by transmission electron microscopy. The modified stabilization treatment produces individual γ' and γ" precipitates and γ'-γ" co-precipitates with average sizes of about 20 nm which are oriented parallel to the $< 001 >$ lattice direction of the γ matrix. There were also observed much bigger individual γ" precipitates with sizes above 50 nm. In addition η precipitates forming at the grain boundaries are detected. The matrix volume fraction after MST is 89 %. During heat treatment at 750°C the small precipitates growth first and are then transformed to η phase. The γ"-phase growths into needles of about 500 nm size. After 5000 h of ageing only one type of precipitates remains, namely η plates embedded into the matrix. The matrix is more enriched in Ni and depleted in Fe as compared with the preceding treatment. The volume fraction of the matrix is close to 93 %.

MM 21.2 Sa 11:15 TU H2038

Variation of Lattice Distortion of Gamma Prime Phase in Creep-deformed Single Crystal Superalloy SC16 with Temperature — •Weye Chen[1], Nora Darowski[2], Ivo Zizak[2], Gerhard Schumacher[2], Helmut Klingelhöffer[3], and Wolfgang Neumann[1] — [1]Humboldt University Berlin, Institute of Physics — [2]Hahn-Meitner-Institute Berlin , Structure and Dynamics — [3]Federal Institute of Materials Research and Testing, Berlin

The lattice distortion of gamma prime precipitates in creep-deformed single crystal superalloy SC16 was investigated by means of high resolution X-ray diffraction technique using synchrotron radiation. The specimens were deformed at 1223 K and 150 MPa to a creep strain of 0.5 temperature. Variations in FWHM can in principle be caused by changes in the size of gamma prime precipitates and by changes in the lattice distortion with temperature. A detailed analysis with respect to the above mentioned aspects led to the conclusion that the effect observed in the present study is essentially caused by temperature-dependent redistribution of internal lattice distortion between gamma prime precipitates and gamma matrix, rather than by changes in precipitate size.

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MM 21.3 Sa 11:30 TU H2038

First-principles prediction of novel ground state structures for the binary systems made of Nb, Ta, Mo, W* — •Volker Blum[1] and Alex Zunger[2] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin — [2]National Renewable Energy Laboratory, Golden, Colorado 80401, USA

The refractory metals Nb, Ta, Mo, and W are the most prominent body-centered cubic transition metals in the periodic system of elements. While the measured mixing enthalpies are negative, implying the existence of some long-range ordered binary crystal structures, the phase diagrams, restricted so far to high-temperature measurements, have revealed only random alloys at high T. It was previously guessed that the ordered structures are ordinary B2 (CsCl type) or $D0_3$ (BiF_3 type), but in principle could be any of the infinite number of other configurations. Combining DFT calculated energies of O(50) configurations for each binary with a "Mixed Basis Cluster Expansion" whose interaction types are chosen by a genetic algorithm search, we derive the energy for *any* bcc configuration. This (Ising-like) functional is then searched to find T=0 ground state structures, and to compute (via Monte Carlo) finite T thermodynamics. The ground states reflect directly the complexity of the underlying interatomic interactions, with the observed absence of high-temperature ordered phases as a consequence. We also predict atomic short-range order in the solid solutions at finite T.

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MM 21.4 Sa 11:45 TU H2038

On the broken-bond model and the pair-potential modelling of alloy surfaces — •Ralf Drautz[1,2] and Manfred Fähnle[1] — [1]Max-Planck-Institut für Metallforschung, Heisenbergstraße 3, 70569 Stuttgart, Germany — [2]Department of Materials, University of Oxford, OX1 3PH, UK

The existence of a surface breaks the symmetry of the bulk material leading in general to an ordering behaviour at the surface which is different from the one of the bulk. We discuss the theoretical modelling of this situation with the cluster-expansion (CE) method [1] and with the many-body potential expansion [2], and we apply these calculational techniques to the system $Ni_{90}Al_{10}(110)$ [1]. It is shown that a broken-bond model which discards the contributions to the CE of clusters with bonds pointing out of the surface and assumes bulk values for the contributions of the remaining clusters may fail badly to describe surface segregation and ordering. The tendency of a minority atom to segregate to the surface of a diluted binary alloy is discussed by use of pair potentials. It is shown that perfectly transferable and hence environment-independent pair potentials [2] in general cannot describe the situation adequately.

[1] R. Drautz, H. Reichert, M. Fähnle, H. Dosch, and J. M. Sanchez, Phys. Rev. Lett. **87**, 236102 (2001)
[2] R. Drautz, M. Fähnle, and J. M. Sanchez, J. Phys.: Condensed Matter **16**, 3843 (2004)

MM 21.5 Sa 12:00 TU H2038

Solidification of Undercooled Intermetallic Forming Systems — •Hamid Assadi[1,2] and Dieter M. Herlach[1] — [1]DLR, Institut für Raumsimulation, 51147 Köln — [2]On leave from: Tarbiat Modarres University, Tehran, Iran

Intermetallics exhibit unique solidification behaviour due to their chemical long-range order. This inclues, for instance, generally slow solidification kinetics, and in some cases, a characteristically sharp change of slope in the corresponding relation between crystal growth velocity and undercooling. The present work uses a phase-field approach to illustrate this behaviour, and further to predict an entire microstructure in an intermetallic forming system. The phase field model is derived from a thermodyanamic formulation, and is assessed qualitatively against the sharp-interface theory of disorder trapping by Boettinger and Aziz (Acta Metall. 1989). A quantitative assessment of the model is provided with respect to the measured growth velocity - undercooling data for various Ni-Al alloys, obtained from electromagnetic levitation experiments.

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