MM 12: Nanostructured Materials IV

Time: Monday 16:45–18:15 Location: H 0107

MM 12.1 Mon 16:45 H 0107

Thermal stability and sinterability of segregation-stabilized nanocrystalline alloys — •Lionel Kroner and Carl E. Krill III — Institut für Mikro- und Nanomaterialien, Universität Ulm, D-89081 Ulm

Although it has recently become possible to calculate the mechanical properties of nanocrystalline materials by means of computer simulation, testing these predictions experimentally has been hampered up to now by the difficulty of preparing nanocrystalline samples in bulk form. Ordinary synthesis routes result in powders or thin films, which might then be compacted to a fully dense state via the application of high pressure and temperature; however, the latter generally induces rapid grain growth, resulting in a coarse-grained final product. A potential strategy for sintering to high density without significant grain growth would be to suppress the driving force for coarsening by adding an atomic species that segregates to the grain boundaries. The effectiveness of this approach has already been demonstrated in nanocrystalline Pd alloyed with Zr [1], but the sinterability of such alloy systems remains to be investigated. We have prepared nanocrystalline Ni-Zr alloys by ball milling and examined the thermal stability and densification as a function of Zr concentration. The microstructural evolution that occurred during pressureless sintering was measured by high-temperature x-ray diffraction, and the density following compaction was determined by Archimedes' method.

[1] C. E. Krill III, H. Ehrhardt and R. Birringer, *Z. Metallkd.* **96** (2005) 1134-1141

MM 12.2 Mon 17:00 H 0107

Influence of grain boundaries on the elastic moduli of nanocrystalline palladium — •Manuel Grewer[1], Jürgen Markmann[1], Rainer Birringer[1], and Walter Arnold[2] — [1]Universität des Saarlandes, FR 7.3 Technische Physik, Campus D2.2, 66123 Saarbrücken — [2]Fraunhofer-Institut für zerstörungsfreie Prüfverfahren, Campus E3.1, 66123 Saarbrücken

Grain boundary stress of nanocrystalline Pd has been determined to be on the order of 1 J/m. There is however only scarce knowledge about the interface elastic moduli of nc materials. We take advantage of the recently discovered room temperature (RT) grain growth of nc-Pd and report about in-situ measurements of the transverse and longitudinal velocities of sound and grain size during RT-growth. We deduce the scaling behavior of the overall elastic moduli and discuss a method that enables to extract interface elastic moduli.

MM 12.3 Mon 17:15 H 0107

Investigation of Natural Aging on Precipitation in Al-Mg-Si Alloys — •Cynthia S. T. Chang, Ingmar Wieler, Nelia Wanderka, and John Banhart — Hahn-Meitner-Institut Berlin, Berlin, Germany

The purpose of this work is to investigate the effect of room temperature storage on microstructural evolution in Al-Mg-Si alloys. Alloy H, with 0.4wt%Mg and 0.4%Si and Alloy F, with 0.6%Mg and 0.8%Si were cast in the laboratory. The alloys were then rolled and solution heat treated (SHT) at 540oC. After SHT, the samples were water quenched and then separated into two batches. One batch was artificially aged at 180oC immediately after SHT, while the other batch was subjected to natural aging before it was aged artificially. Microhardness was measured, and Transmission Electron Microscopy (TEM) and Tomographic Atom Probe (TAP) were used to investigate the microstructures of precipitates at different states. From the hardness measurements, it was found that Alloy F possesses a negative strength response which means that its strength is lower when the sample is naturally aged before artificial aging at 180oC. On the other hand, Alloy H possesses a positive strength response. From the TEM and TAP results, the size, shape and density of precipitates were analysed. The results suggest that the negative and positive responses are related to the density and size of the precipitates after natural aging. This influences the nucleation and growth of precipitates during further aging at 180oC.

MM 12.4 Mon 17:30 H 0107

Charakterisierung der Struktur und Dynamik von Ag-Nanoteilchen in Gläsern mittels EXAFS-Spektroskopie — •Holger Kruth, Jörg Haug, Angelika Chassé und Manfred Dubiel — Universität Halle-Wittenberg, Naturwissenschaftliche Fakultät II, Institut für Physik

Besondere lineare und nichtlineare optische Eigenschaften können durch den Einbau von Metallnanopartikeln in Gläser erzielt werden. Diese Eigenschaften hängen wesentlich von der Partikelgröße (quantum size effect), der Struktur sowie von Metallpartikel-Glas-Grenzflächeneffekten ab. Deshalb wurde die Röntgenabsorptionsspektroskopie (EXAFS) an der Ag-K-Kante eingesetzt, um die Gitterabstände, die statischen und dynamischen Anteile zum Debye-Waller-Faktor sowie die Kumulanten 3. und 4. Ordnung für Ag-Partikelgrößen bis zu 1 nm zu ermitteln. Mit Hilfe dieser Parameter war eine Beurteilung der Unordnung in der Partikel-Glas-Grenzfläche in Abhängigkeit z.B. vom Herstellungsverfahren möglich. Hierbei wurden in die Berechnung des thermischen Ausdehnungskoeffizienten und der Kumulanten anharmonische und quantenmechanische Effekte im Rahmen einer quantenstatistischen Störungstheorie dritter Ordnung einbezogen [1]. Nur so konnten wesentliche Abweichungen im Vergleich zum kompakten Silber für Partikelgrößen unterhalb von 4 nm nachgewiesen werden.

[1] M. Dubiel, A. Chassé, J. Haug, R. Schneider, H. Kruth in Conference Proc. 882, Melville, New York, 407-409, 2007.

MM 12.5 Mon 17:45 H 0107

Initial stages of mechanical alloying of Fe-Cu-powders investigated by Atom Probe Tomography (APT) — •Catharina Wille[1], Malte Schmidt[1], Taláat Al-Kassab[1], Pyuck-Pa Choi[2], and Reiner Kirchheim[1] — [1]Georg-August-Universität Göttingen, Institut für Materialphysik, Göttingen, Germany — [2]Korea Institute of Science and Technology, Nano-Materials Research Center, Seoul, Korea

Mechanically alloyed powders have been commonly used in industrial application (e.g. spray coatings) for several decades due to their outstanding macroscopic properties. Nevertheless the alloying mechanisms in immiscible systems, characterized by a positive heat of mixing, have not been fully understood so far. To elucidate these associated mechanisms a combination of Atom Probe Tomography (APT), Transmission-Electron-Microscopy (TEM) and X-Ray-Diffractometry (XRD) has been employed to the Fe-Cu-system, which serves as a binary model system.

Powders with low concentrations of the respective minority component ranging from 2.5 at.% to 10 at.% have been investigated, both for Fe-rich and Cu-rich materials. Among the studied milling times of 30min to 50h, this talk will put special emphasis on the shorter times, enabling to gain further insight into the early stages of alloying. Additionally, the effects of impurities such as Oxygen and Carbon on the alloying process will be presented and discussed.

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MM 12.6 Mon 18:00 H 0107

molecular dynamic simulations of homogeneous nucleation of zinc from the supersaturated vapour phase. — •Frank Römer and Thomas Kraska — Institute for Physical Chemistry, University Cologne, Germany

We investigate the homogeneous nucleation of supersaturated zinc vapour by non-equilibrium molecular dynamics simulation [1]. Argon is added to the vapour phase, which acts as inert gas thermostat to remove the latent heat from the forming clusters. Our simulations cover a temperature range from 400 K to 800 K and a supersaturation ranging from log(S) = 2 to 11. We compare two methods for the detection of clusters namely the Stillinger criterion based on atom distances only and the ten Wolde-Frenkel cluster definition requiring at least five next neighbours for each atom to be part of a cluster. To obtain the nucleation rates and the critical cluster sizes, we use the so-called threshold method by Yasuoka and Matsumoto [2] and a mean first passage time method by Wedekind et al. [3]. The simulation results show large deviation to the classical nucleation theory. A similar deviation has been found for experimental data in comparison with the classical nucleation theory. In conclusion the experimental data and simulations are in different domains with respect to supersaturation but both deviate consistently from the classical nucleation theory.

[1] F. Römer, T. Kraska, J. Chem. Phys. in press;
[2] K. Yasuoka, M. Matsumoto, J. Chem. Phys. 109, 8451 (1998);
[3] J. Wedekind et al., J. Chem. Phys. 126, 134103 (2007)