saedrische Nahordnung, die kürzlich durch eleastische Neutronenstreuexperimente im Großwinkelbereich bestätigt wurde [2]. Wir berichten über Untersuchungen an unterkühlten Schmelzen von reinem Ni und von Cu-Co Legierungen mit Hilfe der Neutronen-Kleinwinkelstreuung. Die Proben wurden in einem elektromagnetischen Levitationsofen geschmolzen und in-situ auf dem SANS Instrument V4 am HMI, Berlin untersucht. Durch den tiegelfreien Prozess der Schmelze unter hochreinen Bedingungen wurde heterogene Keimbildung unterdrückt, wodurch Unterkühlungen bis zu 300°C erreicht wurden. Im Verlauf der Unterkühlung tritt neben der inkohärenten Flüssigkeitsstreuung ein Kleinwinkel-Streusignal auf, das auf Dichte-Fluktuationen im Nanometerbereich hindeutet. [1] F.C. Frank, R. Soc. A215(1952) 43. [2] T. Schenk, D. Holland Moritz, V. Simonet, R. Bellissent and D.M. Herlach, Phys. Rev. Lett. 89 (2002) 075507.

MM 24 Nanoskalige Materialien III

Zeit: Samstag 14:45–16:00 Raum: TU H111

MM 24.1 Sa 14:45 TU H111

Computersimulation der Kondensation von Nanopartikeln aus der Gasphase — •Ralf Meyer — Département de physique, Université de Montréal, C.P. 6128 succ. Centre-Ville, Montréal (Québec) H3C 3J7, Kanada

Die Bildung von Ni Nanopartikeln aus der Gasphase wird mit Hilfe von Molekulardynamik-Simulationen untersucht. Diese Simulationen zeigen, wie sich zunächst sehr heiße flüssige Nickeltröpfchen bilden, die im weiteren Verlauf kristallisieren und schließlich zu größeren Teilchen agglomerieren. Die strukturellen Eigenschaften der resultierenden Teilchen sind denen von experimentell hergestellten Nickel Nanopartikeln sehr ähnlich. Die Kühlung in den Simulationen erfolgt durch die Wechselwirkung der Nickelteilchen mit den Atomen eines dünnen Argongases. Eine Analyse der Aufteilung der kinetischen Energie zeigt, dass dabei die verschiedenen Freiheitsgrade des Systems unterschiedlich schnell thermalisieren. Die in den Translations- und Rotationsfreiheitsgraden der Teilchen gespeicherte kinetische Energie nimmt deutlich langsamer ab die Energie in den Schwingungsfreiheitsgraden der Teilchen. Insbesondere die überproportional hohe Rotationsenergie könnte dabei einen Einfluß auf die Struktur der entstehenden Teilchen haben.

MM 24.2 Sa 15:00 TU H111

Modeling of the ECAP process: Misorientation evolution — •Ralph Jörg Hellmig[1], Hyoung Seop Kim[2], and Juri Estrin[1] — [1]Institut für Werkstoffkunde und Werkstofftechnik, TU Clausthal, Agricolastr. 6, 38678 Clausthal-Zellerfeld — [2]Dept. of Metallurgical. Eng., Chungnam National University, Daejeon, 305-764, Korea

Using Equal Channel Angular Pressing (ECAP) an ultrafine grained microstructure can be achieved. It has been demonstrated that FEM calculations based on a dislocation density related constitutive model are a suitable method to describe the structure refinement as well as the evolution of mechanical properties and overall texture [1,2]. So far, the evolution of the average misorientation between neigbouring dislocation cells was not included in this model description. A simple extension based on experimental evidences introduced in the FEM code allows to trace the evolution of the average misorientation angle. Results of modeling will be compared with experimental data.
[1] S.C. Baik, R.J. Hellmig, Y. Estrin, H.S. Kim; Z. Metallkd. 94 (2003) 754.
[2] S.C. Baik, Y. Estrin, R.J. Hellmig, H.T. Jeong, H.G. Brokmeier, H.S. Kim; Z. Metallkd. 94 (2003) 1189.

MM 24.3 Sa 15:15 TU H111

Designing tools for ECAP processing — •Mikhail V. Popov, Torbjørn Lamark, Ralph Jörg Hellmig, and Juri Estrin — Institut für Werkstoffkunde und Werkstofftechnik, TU Clausthal, Agricolastr. 6, 38678 Clausthal-Zellerfeld

In recent years Equal Channel Angular Pressing (ECAP) became one of the most important methods for the production of ultrafine grained materials. General ECAP tools are simple in design, but to have really good processing conditions to achieve homogeneous microstructures more advanced tools including features like backpressure or even sliding walls are necessary. In this talk, an introduction on the critical parameters of ECAP processing will be given followed by a discussion of possible solutions for obtaining high performance ECAP equipment.

MM 24.4 Sa 15:30 TU H111

Molecular dynamics investigation of the coalescence of iron nanoparticles — •Norbert Lümmen and Thomas Kraska — Universität zu Köln, Institut für Physikalische Chemie, Luxemburger Str. 116, D-50939 Köln

Coalescence is an important process over the course of the formation of nanoparticles. It significantly influences the properties of the resulting particles. In this work we have investigated the coalescence of iron nanoparticles in the gas phase. Argon has been added in order to reproduce the experimental situation in an inert gas aggregation source (IGA). The heat generated during the coalescence is removed from the system via the inert gas atoms. For the calculation of the interaction between the iron atoms a further development of the embedded atom method for iron taken from the literature has been employed.

The investigation shows that the coalescence of structured clusters evolves via three steps. Each of these steps happens on a different time scale and at different degree of heat exchange with the inert gas. So far such investigations have been performed without an inert gas and therefore the cooling down of the particles during the coalescence has been omitted.

MM 24.5 Sa 15:45 TU H111

Highly ordered nanoparticle arrays with tunable shape, size and spacing — •Yong Lei, Jörg Weissmüller, and Gerhard Wilde — Institute of Nanotechnology, Research Center Karlsruhe, P.O.Box 3640, D-76021 Karlsruhe, Germany

We report an approach to fabricate highly ordered semiconductor or metal nanoparticle arrays with controllable shape, size and spacing. Nanometer-sized discs, hemispheres, hemi-ellipsoids, and conical morphologies have successfully been obtained. The nanoparticle arrays are fabricated on Si or Si/SiO_2 substrates, using ultra-thin alumina membranes as evaporation masks. The shapes and the sizes of the nanoparticles are adjusted by changing the aspect ratio of the apertures of the nanostructured masks and the amount of material deposited through the nanoporous membranes. The size of the arrayed nanoparticles can be adjusted from 10 to 200 nm. The nanoparticle arrays reported here have been applied in some areas, including field emission and electronic devices. In addition, the nanoparticle arrays are well-suited for investigations concerning size-dependent phenomena due to their extremely narrow size distribution.

MM 25 Material Design

Zeit: Samstag 14:45–16:30 Raum: TU H2038

MM 25.1 Sa 14:45 TU H2038

Consolidation Process during Diffusion Bonding in Continuous Al2O3 Fiber-reinforced NiAl Composites — •Hao Chen, Weiping Hu, Yunlong Zhong, and Günter Gottstein — Institute of Physical Metallurgy and Metal Physics, RWTH Aachen, 52056, Aachen, Germany

A theoretical model for solid-state diffusion bonding during the consolidation process of continuous Al2O3 fiber reinforced NiAl composites has been presented. The aim of which was to evaluate the operated mechanisms for consolidation and to determine the optimal hot pressing parameters (time, temperature, pressure). It was found that plastic deformation caused by creep was dominant mechanism in the consolidation process at high temperatures and high pressures. Only in the final collapse of the porosities, the diffusion mechanisms (surface diffusion, volume diffusion and grain boundary diffusion) played a relative important role. The effects of fiber volume fraction and the arrangement of the