

**PS01.07.07 ANALYSIS OF ANISOTROPIC SANS PATTERNS OBTAINED FROM Ni-Al-Mo ALLOYS WITH BIMODAL PARTICLE SIZE DISTRIBUTIONS.** H.A. Calderon, J.G. Caba-As-Moreno, J.J. Cruz, Dept. Ing. Met., E.S.I.Q.I.E.-I.P.N., Apdo. Postal 75-874, Mexico 07738, And J.S. Pedersen Dept. Sol. State Physics, Riso National Lab., Dk-4000 Roskilde, Denmark.

The coarsening kinetics of bimodal distributions of coherent particles in the alloys Ni-14 at.%Al, Ni-10at%Al-5 at.%Mo and Ni-6.5 at.%Al-10 at.%Mo have been investigated by means of small angle neutron scattering (SANS) and by transmission electron microscopy (TEM). Mo has been added to the binary Ni-Al alloys in order to tune the elastic interaction between particles during ripening. In solids, the elastic strain energy can affect the coarsening process of particles, as theoretically predicted by several investigators. The bimodal distributions are created by aging at two different temperatures. Aging at high temperature produces a class of large precipitates in short times. Their coarsening behavior has been investigated by microscopical techniques since they cannot be detected by SANS. Aging at lower temperatures gives rise to the formation of a second set of smaller particles. SANS has been used to determine size, shape and arrangement of particles as a function of the aging time for this set of smaller particles. Single crystalline specimens oriented with the plane (110) parallel to their surface have been used for the SANS measurements. Some of the patterns are markedly anisotropic showing interference peaks along directions [001] and non-circular shapes at large scattering vectors ( $q$ ). This indicates that particles have preferential arrangements in space and that their shape is not spherical. Sequeira et al. [1] analyzed such anisotropic patterns using a technique developed for isotropic patterns [2]. They found large inconsistencies with TEM measurements. In the present case, an evaluation technique for anisotropic patterns has been developed and the results are compared to TEM measurements.

[1] A.D. Sequeira, H.A. Calderon, G. Kostorz, J.S. Pedersen, Acta Metall. Mater. 43, 3427 (1995).

[2] J.S. Pedersen, J. Appl. Crystallogr. 21, 729 (1991).

**PS01.07.08 STUDY OF COHERENCY STRAIN EFFECT ON THE COARSENING IN NI-AL-SI ALLOYS BY NEUTRON TECHNIQUES\*** Haydn Chen, Department of Materials Science & Engineering, University of Illinois, Urbana, IL 61801, G. Muralidharan, MSD, Argonne National Laboratory, Argonne, IL 60439, J. Richardson, IPNS, Argonne National Laboratory, Argonne IL 60439

Superalloys are utilized at a higher proportion of their actual melting point than any other class of broadly commercial metallurgical materials. Ni-based alloys are the most complex, the most widely used for the hottest parts, and to many metallurgists, the most fascinating of all superalloys. Their excellent high temperature mechanical properties are mainly due to the fine precipitation of a variety of phases. Since the commercial alloys are usually complex multicomponent systems, understanding the precipitation phenomena in simple binary and ternary alloy systems is necessary before a full understanding of the commercial variants can be expected. A careful comparison between experimental data and existing precipitation theories is then possible, and more fundamental guidelines can be set to help superalloy design applications. The present study is thus aimed to investigate the kinetics and mechanism of the precipitation process of an ordered  $g'$  phase ( $L1_2$  structure) in Ni-Al and Ni-Si binary alloys as well as in Ni-Si-Al ternary system employing time-resolved small-angle neutron scattering and neutron powder diffraction techniques. The objective of this work is first to provide a unified and comparative view of the precipitation phenomena in two binary systems with opposite signs of lattice mismatch, and secondly, to investigate the effect of lattice-mismatch strain on the kinetic behav-

ior in properly-controlled ternary system. The strain effects on the spatial correlation of precipitates and on the coarsening rates are addressed. Anomalous coarsening rates were observed in the ternary system which is attributed to the coherency strain resulted from the lattice mismatch between the two phases. A plausible mode is described to explain this anomaly.

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**PS01.07.09 LOW-MELTING POINT ORGANIC CRYSTAL STRUCTURES BY HIGH RESOLUTION NEUTRON POWDER DIFFRACTION** Richard M Ibberson, ISIS Facility, Rutherford Appleton Laboratory, Chilton, Didcot, Oxfordshire OX11 0QX, UK

High resolution neutron powder diffraction is a particularly suitable technique for structure solution and refinement of low-melting point organic crystals. Whereas materials that are gas or liquid at ambient temperature pose practical difficulties both in growing single crystals and also in preparing small volume samples for X-ray studies that exhibit a good powder average, low-temperature sample preparation and data collection for neutron powder diffraction experiments is relatively straightforward. These practical advantages and high resolution instrumentation are a powerful combination that enable the precise and accurate determination of moderately complex molecular crystal structures to be performed.

This paper discusses recent examples of *ab-initio* crystal-structure determination and refinement of model methyl-group containing compounds, and the use of such structural data in the calculation of methyl-group rotation potentials for comparison with potentials derived from complementary measurements of tunnelling and librational transitions. Examples discussed will include:

- (a) dimethylacetylene,  $C_2(CH_3)_2$ ; m.p. 241K
- (b) dimethylsulphide,  $S(CH_3)_2$ ; m.p. 175K
- (c) methylfluoride,  $CH_3F$ ; m.p.131K, b.p. 195K.

**PS01.07.10 DIRECT OBSERVATION OF HYDROGEN - DEUTERIUM EXCHANGE IN COBALOXIME CRYSTALS BY NEUTRON DIFFRACTION.** Y. Ohgo<sup>a</sup>, Y. Ohashi<sup>a</sup>, W. T. Klooster<sup>b</sup> and T. F. Koetzle<sup>b</sup>, <sup>a</sup>Department of Chemistry, Tokyo Institute of Technology, Meguro-ku, Tokyo 152, Japan, <sup>b</sup>Chemistry Department, Brookhaven National Laboratory, Upton, New York 119735000

It has been found that the chiral alkyl groups bonded to the cobalt atom in some cobaloxime complexes are racemized on exposure to visible light in the solid-state. To examine the mechanism of crystalline-state racemization we prepared cobaloxime complexes which have deuterium instead of hydrogen bonded to the chiral carbon of the cyanoethyl group and analyzed the crystal structure before and after the photoirradiation by neutron diffraction. The molecular structure before irradiation is shown in Fig. 1.

The structure after irradiation showed that the deuterium, D9, was exchanged with one of hydrogen atom of the neighboring methyl group, H10B. This may suggest quite a new mechanism of the racemization.

Table 1 Crystal data

|                  |           |           |
|------------------|-----------|-----------|
| $a/\text{\AA}$   | 8.686(2)  | 8.750(8)  |
| $b/\text{\AA}$   | 13.516(3) | 13.699(5) |
| $c/\text{\AA}$   | 9.618(3)  | 9.078(8)  |
| $\beta/^\circ$   | 96.92(2)  | 99.06(7)  |
| $V/\text{\AA}^3$ | 1120.9(7) | 1073.4(8) |
| Space Group      | $P2_1$    | $P2_1$    |
| Z                | 2         | 2         |
| Temp.            | 296K      | 15K       |

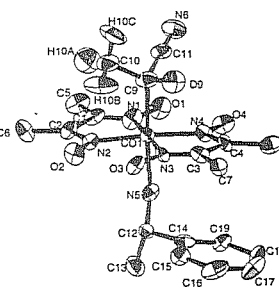


Fig. 1. Molecular structure