

Germany, ²TU Braunschweig, Institut fuer Werkzeugmaschinen und Fertigungstechnik, Langer Kamp 19b, Braunschweig, 38106, Germany, E-mail: katharina.rolfs@hmi.de

Magnetic Shape memory alloys are materials that can potentially substitute giant magnetostrictive systems and piezoelectrical ceramics in actuating devices due to the large magnetically induced strains. It also opens the door to a myriad of other industrial applications. Because of their relatively high operational temperature and the low magnetic fields needed to induce macroscopic strains, Ni-Mn-Ga-single crystals are one of the most common alloys for actuators based on the magnetic shape memory effect. Since the Bridgeman-technique for single-crystal growth is not able to cope with the high vapour-pressure of manganese, a recently developed technique called SLARE (Slag Remelting And Encapsulation) was used for a reliable and repeatable growth of homogeneous single crystals of known composition and low porosity. Using this new method, it is now possible to grow single crystals such as Ni_{49.7}Mn_{29.3}Ga₂₁ of tetragonal martensitic structure (5M) exhibiting a magnetic field induced strain of more than 4% below 170 mT. Since this effect occurs only in the ferromagnetic modulated (5M and 7M) martensitic structures, the application of these materials is still limited by the phase-transition temperature from martensite to austenite, which is now about 65°C in Ni-Mn-Ga. In order to augment the working temperature further, Co-doped Ni-Mn-Ga single crystals have been grown successfully. Up to now a possible working temperature of approximately 120°C has been achieved in Ni_{45.1}Co_{4.9}Mn_{31.9}Ga_{19.1} showing a stress induced (7.5MPa) strain of 1.5%. The stress-strain-analysis and the crystallographic characterization of these promising materials will be discussed here in detail.

Keywords: shape-memory alloys, single crystals growth, alloy development

MS.55.1

Acta Cryst. (2008). A64, C97

Structure of nanomaterials via electron multiple scattering

Michel A Van Hove

City University of Hong Kong, Physics and Materials Science, 83 Tat Chee Avenue, Kowloon Tong, Hong Kong, none, 12345, Hong Kong SAR, E-mail: vanhove@cityu.edu.hk

We have extended to nanostructures the basic theoretical capabilities of surface structure determination by low energy electron diffraction (LEED), by adopting a non-periodic cluster approach and substantially accelerating the computation time for complex structures. Conventional LEED computation times scale as the square or the cube of the number of atoms N whose positions are to be fit to experimental data. In our new method, called NanoLEED, that scaling is reduced to $N \log N$, allowing the solution of much more complex structures, including nanostructures. We describe the application of the new method to an ordered array of buckyballs adsorbed on a Cu(111) surface and to individual silicon nanowires. In the former case, existing experimental approaches can be used since the sample is a periodic extended surface. In the latter case of individual nanostructures, new experimental approaches have been proposed, such as LEED with a convergent beam [1] and LEED with an STM tip as source [2]. The computational method can be readily applied to other structural techniques such as photoelectron diffraction and x-ray absorption fine structure.

I. J.C. Spence, H.C. Poon, D.K. Saldin, *Microscopy and Microanalysis*, 10, 128 (2004)

2. S. Mizuno, F. Rahman, and M. Iwanaga, *Jpn. J. Appl. Phys., Part 2*, 45, L178 (2006)

Funded in part by RGC Grant No. CityU1/02C and CityU Grant No. 9610059.

Keywords: electron scattering, multiple scattering, nanocrystals

MS.55.2

Acta Cryst. (2008). A64, C97

Distinguishing chirality using electron diffraction

Carol J Hirschmugl, Luke Burkholder, Sara Chamberlin, Hin Chuck Poon, Dilano Saldin, Wilfred Tysoe

University of Wisconsin-Milwaukee, Department of Physics, 1900 E Kenwood Blvd, Milwaukee, WI, 53211, USA, E-mail: cjhirsch@uwm.edu

Adsorption of either R- or S-2-butanol chirally modifies a Pd(111). Enantioselectivity has been confirmed by adsorbing either R- or S-propylene oxide as a probe molecule and measuring the resulting coverage of the propylene oxide on the templated surface. This work reveals that low energy electron diffraction I/V curves are different for the R- and S- 2-butanol adsorbates, indicating that in contrast to x-ray diffraction, electron scattering is enantiodifferentiating. A Delay Line Detector Low Energy Electron Diffraction (DLD-LEED) system using a minimal electron dose to collect a series of LEED images as a function of energy has been used to examine the hydrocarbon adsorbate structures for S- and R-2-butanol. Total electron doses of approximately 10^7 electrons are small enough that less than 1% of the adsorbates interact with and are potentially destroyed by the electron beam during the entire collection time of the experiment. The LEED data show that the 2nd order diffraction spots ($\{2,-1\}$ and $\{-1,2\}$) exhibit an asymmetry in the I/V curve that is dependent on the chirality of the adsorbed molecule. This difference disappears for a racemic mixture of adsorbed 2-butanol.

Keywords: chiral recognition, electron diffraction techniques, surface studies

MS.55.3

Acta Cryst. (2008). A64, C97-98

Surface enrichment layers in pressure sensitive adhesive films

Alexander Diethert¹, Stephan V. Roth², Peter Muller-Buschbaum¹

¹TU München, Physik-Department LS E13, James-Franck-Str. 1, Garching, Bayern, 85748, Germany, ²HASYLAB at DESY, Notkestr. 85, Hamburg, 22603, Germany, E-mail: diethert@ph.tum.de

Pressure sensitive adhesives (PSA) are used for many different applications, such as for example adhesive foils or binding materials. A prominent class of PSA films is based on statistical copolymers. Typically, two or three different monomers are combined in the statistical copolymer to balance the different requests of the PSA. The adhesive properties of the PSA films are mainly determined by surface-near regions. However, detailed information about surface structures of such adhesive films is still missing. In the presented work we focus on PSA model systems of statistical copolymers consisting of two different types of monomers. On average our polymer chains are composed of 90% poly(ethyl hexylacrylate) and of 10% of a second monomer which is referred to as the minority component. Different types of monomers are used for the minority component, such as polystyrene, poly(methyl methacrylate) or