

**PS10.03.15 CRYSTAL MODULUS OF POLY(HYDROXY-BUTYRATE)** Jintana Siripitayananon and Teerapol Wongchanapiboon, Biomedical Polymers Research Unit\*, Department of Chemistry, Faculty of Science, Chiang Mai University, Chiang Mai, 50200, Thailand; Timothy M. Nicholson, A. Paul Unwin, Ian M. Ward, IRC in Polymer Science and Technology, University of Leeds, Leeds, UK LS29JT

The crystal modulus of poly(hydroxybutyrate) (PHB) has been measured using changes in the X-ray diffraction pattern of oriented samples under stress. Results obtained below the  $\beta$ -transition temperature give a value of 9 GPa. Two molecular modelling packages, BIOSYM and CERIUS, have been used to predict the full matrix of stiffness coefficients for PHB and hence, *via* the aggregate model, the properties of a uniaxial fibre. The modulus along the chain direction compares well with the experimental value. Both packages predict a high transverse modulus and this is shown to be consistent with the measured modulus of the isotropic polymer on the basis of the aggregate model.

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**PS10.03.16 PARTICLE SIZE AND STRAIN MEASUREMENT IN RHENIUM POWDER BY MEANS OF THE WARREN-AVERBACH METHOD.** J.L. Garin, R.L. Mannheim, Department of Metallurgical Engineering, J.A. Costamagna, Department of Chemistry, Universidad de Santiago de Chile, Casilla 10233, Santiago, Chile

Crystallite size, crystallite size distribution and microstrain in polycrystalline rhenium samples, were evaluated from diffraction peak broadening.

The material used in this research was rhenium powder produced by reduction of ammonium perrhenate ( $\text{NH}_4\text{ReO}_4$ ) under hydrogen flux inside a tubular furnace, at various temperatures in the range of 673 to 1273 K. Depending upon the process temperature, variable amounts of hydrogen, nitrogen and oxygen remain in the material causing large line broadening. Powder data were collected at room temperature with a SIEMENS D5000 diffractometer equipped with a graphite diffracted beam monochromator, using a normal Cu tube. Measurements of particle size distribution and strain made use of the (101) and (202) powder diffraction profiles. The standard powder sample for the determination of instrumental broadening was obtained from rhenium produced at 1273 K. All experimental profiles were modeled by use of Pearson VII functions, while the calculations were based upon the Warren-Averbach theory, and carried out with the programs PROFILE and WIN-CRYSIZE distributed by SIEMENS.

The particle size varied from 3 nm (673 K) to 80nm (1123 K); no variations were observed at higher reduction temperatures. On the other side, the microstrain changed from an average value of  $8.7 \times 10^{-3}$  to  $0.8 \times 10^{-3}$ , with no further changes at higher temperatures. The overall results are in close agreement with the contents of hydrogen, nitrogen and oxygen impurities, which remain interstitially dissolved in the hexagonal structure of the metal.

**PS10.03.17 NEAR-EDGE AND FINE STRUCTURE OF TITANIUM OXIDES.** Se Ahn Song(1), Jae Cheol Lee(1), K. Yu. Pogrebitsky(2) and O.A. Usov(2). 1 Samsung Advanced Institute of Technology, P.O.Box 111, Suwon, 440-600, Korea; 2 Ioffe Phys.-Tech.Institute, Polytechnical str., 26, St. Petersburg, 194021, Russia.

The X-ray absorption spectra (near-edge, fine structure) of  $\text{TiO}_2$  and related oxides were measured by total electron yield (TEY) mode at laboratory device, using channeltron. The powder was checked by X-ray diffraction at RT to assure the rutile structure and its unit cell parameters were determined. The average size of crystallites was found by SEM to be within the range of absorption length of material. The effect of particle size for such prepared samples on the TEY amplitude is expected to be negligible. The threshold and minimum XAFS energy were fitted to provide small oscillations XRD functions at low R-space distances. The energy positions of near-edge peaks defined as negative minima of second derivatives are shown to be in a good agreement with the transmission XAFS spectra for  $\text{TiO}_2$ [1] and  $\text{PbTiO}_3$ [2]. The possibility of multi-electron excitations in the structure is also discussed. The structure parameters of Ti first coordination sphere were calculated by fitting theoretical FT-XAFS data to experiment alone in the specified R-space region. The values of Ti-O distances and the mean squared displacements were found to be in good agreement with the X-ray diffraction and transmission XAFS data, however some differences being attributed to the surface strain effects.

1. B. Poumellec et al, Phys.Rev.,B35(1987)2284-94.
2. N. Sicron et al, Phys.Rev.,B50(1994)13168-80.

## Materials IV Aperiodic Structures & Incommensurate Phases

**MS10.04.01 X-RAY DIFFRACTION STUDIES ON DIFFUSE SCATTERING IN SINGLE QUASICRYSTALS.** F. Dénoyer, Laboratoire de Physique des Solides, Associé au CNRS, Bâtiment 510, Université Paris-Sud, 91405 Orsay Cédex, France.

In addition to the diffraction peaks observed in icosahedral and decagonal phases, X-ray diffraction patterns reveal diffuse scattering which also exhibits icosahedral (F. Dénoyer, G. Heger, M. Lambert, J.M. Lang, P. Sainfort, J. Physique 48 (1987) 1357-1361, P. Donnadiou, F. Dénoyer submitted) or decagonal symmetry (F. Frey, W. Steurer, J. of Non-Cryst. Solids, 153&154 (1993) 600-605, M. Fettweis, P. Launois, F. Dénoyer, R. Reich, M. Lambert, Phys. Rev. B49 (1994) 15573-15587, M. Fettweis, P. Launois, R. Reich, R. Wittmann, F. Dénoyer, Phys. Rev. B51 (1995) 6700-6703). The origin of this diffuse scattering is of interest since it may allow to understand the mechanism of formation of quasicrystals.

Spherical shells (or arcs) of diffuse scattering in electron and X-ray diffraction patterns seem to be a characteristic of icosahedral phases. These diffuse features have been interpreted as the result of an intrinsic packing disorder of the alloy structures, most of the models being based on dense randomly packing distributions of icosahedral clusters of atoms (A.I. Goldman, C.A. Guryan, P.W. Stephens, J.M. Parsey, Jr., G. Aeppli, H.S. Chen, F.W. Gayle, Phys. Rev. Lett. 61 (1988) 1962-1965, J.L. Robertson, S.C. Moss, J. of Non-Cryst. Solids 153&154 (1993) 77-82, P.C. Gibbons, K.F. Kelton, J. of Non-Cryst. Solids 153&154 (1993) 165-171, M.E.J. Newman, C.L. Henley, M. Oxborrow, Phil. Mag. B71 (1995) 991-1013).

In decagonal alloys (F. Frey, W. Steurer, J. of Non-Cryst. Solids, 153&154 (1993) 600-605, M. Fettweis, P. Launois, R. Reich, R. Wittmann, F. Dénoyer, Phys. Rev. B51 (1995) 6700-6703, M. Fettweis, PhD thesis Université ParisXI, France (1994)), localized diffuse scattering disappears above 800°C. At room temperature, their shapes depend on the chemical composition of the alloy and are quite different according as the sample is in a decagonal metastable quenched quasicrystalline state or in a stable decagonal-like microcrystalline state.