**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 orientated samples under stress. Results obtained below the b-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, Castilla 10235, Santiago, Chile

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

The material used in this research was rhenium powder produced by reduction of ammonium perrenenate (NH4ReO4) 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 50 nm (1123 K); no variations were observed at higher reduction temperatures. On the other side, the microstrain changed from an average value of 8.7x10^{-3} to 0.8x10^{-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. Pogrebitskyy(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, Politechnical str., 26, St. Petersburg, 194021, Russia.

The X-ray absorption spectra (near-edge, fine structure) of TiO2 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 material structure and its phase composition. The possibility of multiplet 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.


**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, Associated au CNRS, Bâtiment 510, Université Paris-Sud, 91405 Orsay Cédex, France.

