20-Industrial Crystallography

20.01 – Aspects of Industrial Crystallography

MS-20.01.01 NEUTRON DIFFRACTION FOR NON-DESTRUCTIVE STRESS/STRAIN MEASUREMENTS IN INDUSTRIAL DEVICES by Hans Georg Priesmeyer*, Institut fur Reine und Angewandte Kernphysik der Universitat Kiel, Otto-Hahn-Piatz 1, 24118 Kiel, Germany

High resolution neutron diffraction is becoming diffraction is becoming widely used as a non-destructive tool to investigate three-dimensional stress fields in polycrystalline metals and ceramics. Lattice strains can be derived from Bragg peak positions measured with an accuracy better than 1:104. Both crystal and time-of-flight diffractometry are used to perform the measurements, as will be demonstrated by examples. New instrumental developments like the european PREMIS project at ISIS/England, the Fourier correlation spectrometer FSS at Geesthacht/Germany, and the energy-dispersive Neutron Transmission Stroboscope at LANSCE/United States, will be introduced. Recent results on industrial devices will be presented and discussed.

MS-20.01.02 POWDER DIFFRACTION IN PATENTS. By S.E.Tarling, British Gas plc, Gas Research Centre, Ashby Road, Loughborough LE11 3QU, UK

MS-20.01.03 INDUSTRIAL USES OF SYNCHROTRON RADIATION by R.J.Cernik*, Daresbury Laboratory, Warrington WA44AD, UK

There is currently a worldwide trend towards performing more applied or "near market" research in higher education establishments and central facilities. This talk will focus on some of the more successful applications of synchrotron radiation to the solution of some applied industrially relevant problems. There examples will include applications in lithography for the manufacture of miniature mechanical parts, the solution of organic crystal structures from powder diffraction which are relevant to the pharmaceutical industry, the study of ceramic using time resolved diffraction, how catalytic activity can be studied in situ using energy dispersive diffraction, and how protein crystallography was be used to identify
a target for the possible treatment of trypanosomiasis.
With new generation sources being built significant gains in flux will be possible this will reduce the time for a powder diffraction scan, for example, from 4 to 5 hours to a few minutes. Similar reductions in time for EXAFS and other synchrotron based techniques offer exciting possibilities for future industrial and "near market" research.

MS-20.01.04 APPLICATIONS OF SMALL-ANGLE SCATTERING by G.Kostorz*, Inst. of Applied Physics, Swiss Federal Institute of Technology (ETH) Zurich, Switzerland

Small-angle scattering of x-rays and neutrons is a versatile tool in the study of defect agglomeration and phase separation in materials, resolving inhomogeneities of dimensions ranging from about 1nm to more than 100nm. Some characteristic results on vacancy agglomeration during fatigue and on the decomposition of Al and Ni alloys will be presented. The scattering from phase separated systems will be discussed in the light of current theoretical concepts of nucleation and growth, spinodal decomposition, scaling laws and elastic interactions of precipitates.

MS-20.01.05 ROUTINE, RAPID, NON-DESTRUCTIVE ANALYSIS OF SEMICONDUCTOR WAFER SUBSTRATES BY REFLECTION ASYMMETRIC CRYSTAL X-RAY TOPOGRAPHY. By I. C. Bassignana* and D. A. Macquistan, Advanced Technology Laboratory, Bell-Northern Research Ltd., P.O. BOX 3511 Station C, Ottawa, Ontario K1Y 4H7, Canada.

Crystal defects, such as low angle grain boundaries and included mosaic crystals, present in single crystal semiconductor substrate wafers are known to adversely affect the yield and performance of devices fabricated directly on the substrates. Asymmetric crystal topography (ACT), a high-resolution, double crystal x-ray technique which requires no special sample preparation, has been adapted to topograph large single crystal wafers (75mm diam.) by using a very large area (100mm diam.) Si(111) first crystal, with a high magnification ratio (40X). This extensive study shows that reflection topographs of entire wafers can be routinely acquired by this non-scanning method in less that 30 min. using a conventional x-ray source (12kW). The device-quality substrates studied include: Si, used in all types of electronic devices; GaAs and InP, used in opto-electronic and high-speed devices; and synthetic single crystal quartz, used for surface acoustic wave devices.

A serious environmental contaminant in semiconductor manufacturing is dust. In order to render the ACT technique totally non-destructive a container has been developed which is transparent to x-rays but which is entirely compatible with semiconductor processing. The container insures that wafers can be removed from the production line for x-ray testing and returned to it without compromising cleanliness.

MS-20.01.06 CRYSTALLOGRAPHY IN THE PHARMACEUTICAL INDUSTRY by T.Skarzynski*, Glaxo Group Research Ltd., Greenford Road, Greenford, Middlesex UB6 OHE, UK

Rational,structure-based design of novel compounds as potential drugs has become a reality. Crystallography plays an increasing role in the process providing structural information on the biological receptors and the ligand-receptor complexes. New techniques of X-ray data collection, accessibility of powerful computers and improved software packages contribute to the rapid increase of structural data available researchers.
An overview of the current crystallographic techniques relevant to the drug discovery process will be given.
HIV protease provides a good example of the use of structural information in the design of potent, highly specific inhibitors that are of potential value as drugs against AIDS. Results of our studies that allowed optimization of lead compounds through an iterative cycle of protein crystallography and medicinal chemistry will be presented.

