consisting of predominantly α-Ti ($P6_3/mmc$) [1]. The Ti-6Al-4V rod was machined using both conventional and high-pressure jet–assisted methods. The depth profile of residual stress was measured using x-ray diffraction. It was found that the compress residual stress is higher and the deeper under which the compress residual stress exists, for sample cut by high-pressure jet–assisted than for sample cut by conventional method [2].

Using transmission electron microscopy the cross-section of the surface layer was found to consist of a thin outer layer with nano-sized crystals (~10 nm) and the substrate of large grains with very high density of dislocations. Electron diffraction reveals that the nano-sized outer layer is highly textured. Furthermore, the study shows that the nano-sized layer has twice the thickness for the high-pressure jet–assisted cut sample (~1,000 nm) than for the conventionally cut sample (~500 nm). This shows that high-pressure jet–assisted cutting resulted in a thick and highly modified outer layer and provides an explanation for the large and deep compressed residual stress after high-pressure jet–assisted cutting of Ti-6Al-4V.

[1] PDF File No.44-1294. [2] Vosough M., Liu P., Svenningsson I., *Mat. Sci. Forum*, 2005, **490-491**, 545-551.

Keywords: titanium alloy, residual stress, metal cutting

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New Tools to Integrate Data Analysis and Data Collection at SSRL: Web-Ice

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Recent developments in automation at the Stanford Synchrotron Radiation Laboratory Macromolecular Crystallography beamlines have been driven by the needs of the Structural Genomics projects and feedback from the user community. Current capabilities at all beamlines include automated sample mounting and centering; crystal screening; fluorescence scan measurements and analysis; and wavelength changes at side stations with automatic table motion to track the beam. These features are implemented on the beamline control software program Blu-Ice.

The most recent software developments at SSRL aim at integrating data analysis and beamline hardware to the point where only minimal input by the user will be required to carry out a complete experiment. In order to facilitate remote access to the experiment, the software is accessible remotely through a web-browser interface known as Web-Ice. Web-Ice currently provides tools to view diffraction images as they are being collected; analyze the diffraction pattern and display statistics (such as number of spots, shape, diffraction strength, etc.) and autoindex and calculate a strategy to maximize data completeness based on two images selected by the user.

The next Web-Ice release will include a crystal screening interface to analyze and score images from multiple samples. Ultimately, the software will fully integrate data analysis and beamline control software for automated data collection.

Keywords: data collection, data analysis, automation

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Study of Micro Structural Defect Parameters in Nickel Dispersed Silica Nano Composites by Warren-Averbach Method and Modified Rietveld Technique

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Detailed Fourier line shape analysis has been performed on the X-ray diffraction profiles of Nickel dispersed silica nano composites, SiO_2-Ni (Wt % Ni-7.5 : Sample I, Ni-10 : Sample II, Ni-15 : Sample III, Ni-20 : Sample IV and Ni-25 : Sample V) by employing Warren-Averbach and modified Rietveld techniques.

The nickel dispersed silica nano composites were prepared through sol-gel route from a homogeneous solution of tetraethyl ortho silicate (TEOS), C_2H_5OH, required amount of $NiCl_2 . 6H_2O$,

$C_6 H_{12}O_6$ and water. The mixture was left at room temperature for gelling. The gel samples thus prepared were washed, dried and used for X-ray analysis.

The micro structural parameters like domain size, micro strain within the domains, deformation stacking fault densities (Intrinsic $\alpha^{/}$, Extrinsic $\alpha^{//}$ and Twin fault β) and dislocation density ρ were evaluated by Fourier line shape analysis taking silicon as standard for instrumental broadening correction. It has been observed from these two analyses that the $\alpha^{/}$ and $\alpha^{//}$ faults are totally absent whereas the twin β has significant presence. It has also been found that the β initially increases up to Sample III and then decreases. This is an observation on twin fault variation with Ni content in this SiO_2 - Ni nano composite system.

Keywords: nano crystals, defect analysis, diffraction

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Synchrotron XRD Study of ZrO_2-CeO_2 Nanopowders Synthesised by Gel-combustion

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Zirconia-ceria solid solutions are being widely investigated due to their excellent mechanical and catalytic properties. For example, these materials are extensively used as promoters in three-way catalysts.

In this work, the crystal structure of nanocrystalline ZrO_2-CeO_2 solid solutions, synthesised by a pH-controlled nitrate-glycine gel-combustion process, has been studied by using a high-intensity synchrotron X-ray diffractometer (D12A-XRD1 beamline of the LNLS, Brazilian Light Facility). Several weak Bragg peaks of the tetragonal phase, which correspond to forbidden reflections in the case of a perfect cubic fluorite structure, were detected. By determining the integrated intensity of the strongest of these reflections, (112), as a function of the CeO_2 content, the tetragonal-cubic phase compositional boundary was established to be at (85±5) mol% CeO_2. For a CeO_2 content up to (68±2) mol%, we identified a tetragonal phase with $c/a > 1$, whereas, in the range between 68 and 85 mol% CeO_2, the existence of a tetragonal phase with $c/a = 1$ and oxygen anions displaced from their ideal positions in the cubic phase (keeping the tetragonal symmetry) was verified. Finally, solid solutions with CeO_2 contents higher than 85 mol% exhibit the cubic fluorite-type phase.

Keywords: synchrotron powder diffraction, zirconia-ceria, nanocrystalline materials

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Characterization of Individual Zincoxide Nano-belts by using X-ray Nano-Diffraction Technique

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Nano-structures, such as wires, rods, belts and tubes, whose lateral dimensions fall in the range of 1 to 100 nm, have received growing interests due to their outstanding proprieties and their potential applications in electronic and biological fields. The development of these new structures into future nano-devices crucially depends on the development of new characterization techniques and theoretical models for a fundamental understanding of the relationship between the structure and properties [1].

X-ray diffraction technique has been successfully applied for characterization of bulk or powder nano-structured materials, where useful information, such as crystallite size distribution, crystallite