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 NiCl₂ 6H₂O,

 C_6 H₁₂O₆ 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 α' , Extrinsic α'' 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 α' and α'' 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 SiO₂ - Ni nano composite system.

Keywords: nano crystals, defect analysis, diffraction