X-Ray Line Profile Analysis of TiO_2 nano-powders

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INTRODUCTION

Research takes dedication, hard work and a time commitment. This summer I have learned the ups and downs of researching. While researching can be fulfilling in the end goal, it can be tedious in terms of what may need to be done to your data or the materials in order for you to come to a conclusion. In working in the laboratory with Dr. Iuliana Cernatescu, I have gained a new appreciation for researchers and their time spent on difficult projects.

Line Profile Analysis was at the heart of my summer research. Researching three nano-powders consumed much of the summer and made it difficult in trying to find some type of correlation between the three. Although I did not get a chance to finish the project in full, Dr. Cernatescu and I started the project off with success.

PROCEDURE

The experiment started with preparing the samples of the TiO_2 nano-powders. The samples were prepared in the laboratory. Using the sample containers of the x-ray diffractometer, three samples were prepared for testing. After the samples were prepared and checked for consistency, each sample at one time was placed in the machine for an extensive period of time ranging from 24 to 44 hours, and did repetitive analysis over the period of time. The machine tested each sample at the angles from 25 degrees to 140 degrees. The machine collected the data for each run.

The major part of the project involved the manual analysis of the data. Once the data has been collected, the diffraction peaks data must be reviewed in order to determine the diffraction peaks that can be used in the analysis and the peaks that should be re-tested in order to get rid of x-ray background. Once all retest have been done, the diffraction data can be used in order to develop a Williamson-Hall plot and perform the Warren-Averbach method which will both determine an average crystallite size. These two can only be done if the data is transformed into its proper coordinates and calculated to reveal such values as the corrected (due to instrumental effects) full-width at half maximum and integral breadth. Once these steps are done, line profile analysis can be done to see if the data that has been collected shows the characteristics of the nano-powder like the average area, average strain, strain and shape.

RESULTS AND DISCUSSION

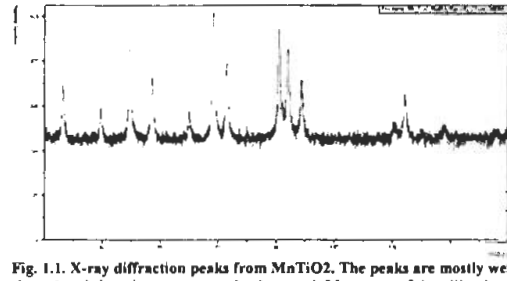

Fig. 1.1. X-ray diffraction peaks from MnTiO2. The peaks are mostly well-shaped and there is no apparent background. Many sets of data like the above were collected by the x-ray diffractometer.

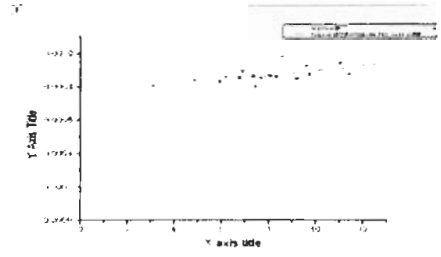

Fig. 1. 2. Williamson-Hall plot for the full-width at half maximum (FWHM) of TiO2. The y-intercept is the average crystallite size and the slope is the micro-strain.

CONCLUSION

No final conclusion could be reached at the moment due to the $SiTiO_2$ data being unavailable. The average crystallite size has been determined for the TiO_2 and $MnTiO_2$ as well as the strain and size distribution. Currently, there are no noticeable variances between the base and doped nano-powders. All powders look spherical.