Modified Scherrer equation to calculate crystal size by XRD with high accuracy, examples Fe_2O_3, TiO_2 and V_2O_5

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Abstract:

~~One of the best parameters~~A key parameter in the analysis of compounds and the study of their physical, chemical, and mechanical properties is the knowledge of the crystal ~~crystal~~ size. There are two common techniques for determining ~~crystal~~ this size: transmission electron microscopy (TEM) and Brunauer- Emmett-Teller theory (BET). These methods are ~~time~~ time-consuming and ~~also~~ expensive~~,~~; ~~therefore~~ thus, the calculation of ~~crystal~~ this size by X-ray diffraction is proposed. There are several methods ~~to~~ for ~~calculate~~ calculating the crystal ~~crystallite~~ size by X-ray diffraction, but not all peaks were considered and the errors were very large. In this study, the ~~Modified~~ modified Scherrer method for TiO_2 and V_2O_5 powders is explained as examples, and the proposed method is applied to each crystallite compound. Furthermore, the steps to be applied to determine the values are clearly defined by the X'Pert software. In addition, the comparison with TEM and BET is discussed in detail. ~~The result is that the~~According to the results, ~~Modified~~ modified Scherrer method has high accuracy and agreement with the ~~analyses of~~ TEM and BET analyses. ~~Therefore~~Thus, ~~the Modified Scherrer~~this method is proposed for ~~the calculation of~~calculating each crystalline compound ~~because~~ as it has high accuracy, XRD analysis is available and cheaper. ~~It is worth mentioning~~Note that the calculation process using the ~~Modified~~ modified Scherrer method is corresponded for any crystalline material.

1. Introduction

Materials can be divided into two categories: crystalline and amorphous. Of course, no material is 100% crystalline. There are sharp and well-defined peaks in the X-ray diffraction (XRD) diagram of materials that exhibit a crystalline order. The XRD diffraction pattern contains sharp peaks indicating the formation of a crystalline phase [1]. In order to study the structural, magnetic, optical, mechanical, and electrical properties of each composition, knowledge of the crystal ~~crystal~~ size is essential [2],[3]. Crystal ~~Crystallite~~ size is a measure of the size of the coherently diffracting domains. Because of the formation of polycrystalline aggregates, the crystal ~~crystallite~~ size of ~~the~~ particles is generally not identical to the particle size. The crystal ~~crystallite~~ size affects the Bragg peak, increases the peak width and intensity, and shifts the position of the 2θ-peak accordingly [5],[6]. XRD is used for primary characterization of material properties such as crystallite structure and crystal ~~crystallite~~ size [7]. For example, XRD can provide useful information on the extent to which the surface treatment of an element has affected the mass of the material. It is possible to use XRD in a thin film mode, with very small acceptance angles to derive some surface information, but in general it must be considered a

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