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PROFILE ANALYSIS OF THE X-RAY DIFFRACTION PATTERN OF HYDROTHERMALLY SYNTHESIZED NaL ZEOLITE: DIFFRACTION PEAK PARAMETERS AND FWHM CHARACTERISTICS

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Abstract: This study presents a profile analysis of the X-ray diffraction pattern of hydrothermally synthesized NaL zeolite. The analysis was performed to characterize individual diffraction reflections and evaluate the structural ordering of the crystalline framework. The principal parameters of the diffraction peaks, including 2θ position, interplanar spacing (d), intensity, integral intensity, full width at half maximum (FWHM), and profile asymmetry, were determined using profile fitting. The obtained results demonstrate that the principal reflections exhibit well-defined profiles and relatively small FWHM values, indicating a high degree of crystallinity and structural ordering. Profile analysis also enabled the resolution of partially overlapping reflections and more reliable determination of their individual parameters. The results demonstrate

the usefulness of peak profile analysis for detailed characterization of the crystalline structure of NaL zeolite.

Keywords: NaL zeolite; LTL framework; X-ray diffraction; profile analysis; diffraction peaks; FWHM; crystallinity; structural ordering.

INTRODUCTION

X-ray diffraction (XRD) is a widely used technique for characterizing the crystalline structure of zeolites and for identifying structural features that influence their functional properties [1-2]. While conventional XRD analysis mainly focuses on the positions and relative intensities of diffraction reflections, detailed analysis of the peak profiles provides additional information about the structural quality and ordering of crystalline materials [3-5].

Profile analysis enables individual diffraction maxima to be mathematically separated and characterized using parameters such as peak position (2θ), interplanar spacing (d), intensity, integral intensity, full width at half maximum (FWHM), and profile asymmetry. These parameters provide useful information about the degree of crystallinity, crystallite perfection, and possible peak overlap within the diffraction pattern [3, 5].

For NaL zeolite with an LTL-type framework, detailed characterization of individual reflections is particularly useful because closely spaced diffraction maxima may partially overlap in the experimental pattern. Therefore, the application of profile analysis can provide more reliable information than conventional qualitative interpretation of the diffraction pattern. The aim of this study was to analyze the principal diffraction maxima of hydrothermally synthesized NaL zeolite and to evaluate their profile parameters, with particular emphasis on FWHM and the quality of the crystalline structure.

METHODOLOGY AND MATERIALS

A hydrothermally synthesized NaL zeolite obtained from chemically pure reagents was used as the investigated material. The synthesis procedure was described in detail in a previous study [4-5]. The present work focused on the quantitative analysis of the X-ray diffraction peak profiles of the synthesized material.

X-ray diffraction measurements were performed using an automated powder diffractometer with monochromated CuKα radiation (λ=1.5406 Å). The diffraction pattern was recorded over the 2θ range of 3-60° with a step size of 0.02°, at an accelerating voltage of 40 kV and an X-ray tube current of 15 mA.

The experimental diffraction pattern was processed using X'Pert HighScore Plus software. Profile fitting was applied to resolve individual and partially overlapping reflections. For the principal diffraction maxima, the 2θ position, interplanar spacing (d), maximum intensity, integral intensity, FWHM, and profile asymmetry coefficient were determined. The obtained parameters were used to compare the individual reflections and to evaluate the degree of structural ordering and crystallinity of the NaL zeolite.

RESULTS AND DISCUSSION

The profile analysis of the X-ray diffraction pattern provided detailed information on the individual diffraction maxima of the hydrothermally synthesized NaL zeolite. In contrast to conventional qualitative XRD analysis, profile fitting made it possible to determine the principal parameters of individual reflections, including their positions (2θ), interplanar spacings (d), maximum and integral intensities, FWHM values, and profile asymmetry coefficients. The main results of the profile analysis are summarized in Table 1.

The diffraction maxima are distributed mainly within the low- and medium-angle regions and correspond to the characteristic reflections of the LTL-type framework. The determined 2θ values and corresponding interplanar spacings are consistent with

the characteristic diffraction features of NaL zeolite. The presence of several closely positioned reflections demonstrates the importance of profile fitting for their reliable separation and individual characterization.

The intensity characteristics of the reflections provide information about the degree of development of the crystalline structure. The most intense diffraction maxima make the largest contribution to the overall diffraction pattern and indicate a well-developed long-range order within the aluminosilicate framework. The combination of high peak intensity and well-defined peak profiles is consistent with the high crystallinity of the synthesized NaL zeolite.

An important parameter obtained from the profile analysis is the full width at half maximum (FWHM). The principal reflections are characterized by relatively small FWHM values, indicating narrow and well-defined diffraction profiles. Such peak characteristics are generally associated with a high degree of crystalline ordering and good crystallite perfection. The absence of pronounced broadening of the principal reflections also indicates that significant structural disorder is not evident from the diffraction profiles.

Table 1. Main parameters of the most intense diffraction maxima of hydrothermally synthesized NaL zeolite obtained by profile analysis.

№	2θ, °	d, Å	Height, cps	FWHM, °	Integral intensity, cps·°	Integral width, °	Asymmetry
1	7.187	12.29	52178	0.149	9437	0.181	3.4
2	10.151	8.7068	40227	0.144	7132	0.177	2.26
3	12.437	7.1112	21604	0.15	3921	0.182	2.07
4	16.088	5.5047	18334	0.155	3414	0.186	2.8
5	21.622	4.1068	37463	0.145	7754	0.207	1.5
6	23.948	3.7129	56077	0.159	11921	0.213	2.2

7	26.075	3.4146	13647	0.171	2596	0.19	2.2
8	27.081	3.29	50183	0.159	10285	0.205	2.6
9	29.899	2.986	59063	0.16	12556	0.213	2.18
10	34.139	2.6243	38943	0.165	8269	0.212	2.66
11	44.107	2.0516	9366	0.177	2305	0.246	1.98
12	52.529	1.7407	12979	0.182	3434	0.265	1.79

The analysis of individual reflections is particularly important in regions where neighboring peaks partially overlap. Conventional measurement of peak height alone may not provide reliable parameters for individual reflections in such cases. Profile fitting allows the overlapping contributions to be separated mathematically and therefore provides more accurate values of the position, intensity, and width of individual peaks. This feature is especially useful for detailed comparison of the structural characteristics of synthetic zeolites.

The profile asymmetry coefficients provide additional information about the shape of individual diffraction maxima. For the principal reflections, the profiles are generally close to symmetric, indicating that pronounced distortions of the diffraction peaks are not observed. Minor deviations from ideal symmetry may result from partial overlap of neighboring reflections or from characteristics of the instrumental profile. However, these deviations do not prevent reliable determination of the principal diffraction parameters.

Overall, the profile-analysis results demonstrate that the hydrothermally synthesized NaL zeolite possesses well-defined diffraction maxima, relatively narrow peak profiles, and a high degree of structural ordering. The quantitative parameters obtained from the individual reflections provide more detailed information about the crystalline structure than conventional qualitative XRD analysis and can be used as a basis for further investigation of the relationship between the structural characteristics of NaL zeolite and its functional properties.

CONCLUSION

The profile analysis of the X-ray diffraction pattern provided detailed quantitative information on the principal diffraction maxima of the hydrothermally synthesized NaL zeolite. The determined 2θ positions, interplanar spacings (d), intensities, integral intensities, FWHM values, and asymmetry coefficients confirmed the well-defined character of the main reflections and the high degree of structural ordering of the crystalline framework.

The relatively small FWHM values of the principal reflections indicate a well-crystallized material with good crystallite perfection and no pronounced peak broadening associated with significant structural disorder. The profile-fitting procedure also enabled the reliable separation and characterization of partially overlapping reflections.

Thus, the obtained results demonstrate that X-ray diffraction profile analysis is an effective approach for quantitative characterization of the crystalline structure of NaL zeolite, providing information beyond conventional qualitative phase identification. The determined peak parameters can be further used to investigate the relationship between the structural characteristics and functional properties of LTL-type zeolites.

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