Indexing of Laue Back Reflection for Quartz Crystal and Singularity Evaluation of Zn Metal Thin Film

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Abstract

Laue back reflection patterns for quartz crystal are indexed by using Orient Express- program to simulate orientation of single crystals from assignment of principle zones. An oriented quartz single crystal was used as a substrate to deposit Zn metal by controlled thermal evaporation to achieve single crystal films of Zn that are subsequently evaluated by x-ray powder diffraction.

Keywords
Indexing of Laue
Quartz Crystal

Article info
Received:
Accepted: Fab
Published: Dec.

فهرسة صور لاوي للانعكاس الخلفي لبلورة الكوارتز وتقييم أحادية غشاء الزنك

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الخلاصة

تم فهرسة صور لاوي للانعكاس الخلفي لبلورة الكوارتز باستخدام برنامج Orient Express لمحاكاة التوجيه في البلورات الأحادية بتعيين الانطقة الرئيسية. استخدمت بلورة أحادية موجهة للكوارتز كأرضية لترسيب معدن الزنك بالتبخير الحراري المسيطر للوصول إلى أغشية رقيقة أحادية التوجيه للزنك والتي جرى تقييمها بواسطة حيود الأشعة السينية للمسحوق.

Introduction

Quartz is a single crystal of silicon dioxide commonly used in an important electronic components of digital equipment such as; mobile communication, optic communications, video equipment and PCs as a precise source of electrical signal [1,2]. Ease of indexing of single crystals by the simulation of Laue pattern from the basic crystal structure data is done efficiently by an Orient Express- program [3]. Thin films deposited by controlled evaporation procedure on single crystal substrates are known to exhibit structure and orientation similar to that of the substrate [4-9] but the major challenge still remain in large scale of thin film based devices [5,10]. The aim of this work is to index Laue x-ray patterns of quartz single crystals and to check the singularity of the Zn metal thin film deposited on quartz.

Experimental

1. Back reflection pattern photography technique

A constructed flat-film Laue camera was used to record diffraction from the crystal in the back reflection region. The crystal of unknown orientation was placed 3cm away from x-ray film. A 0.3 pinhole collimator was used to define the incident x-ray beam. The diffraction pattern was obtained from unfiltered x-ray beam emitted by Cu target at 40 kv and 20 mA on x-ray generator. A typical Laue diffraction pattern for the quartz crystal is obtained in (Fig.1a).

2. Thin Film Evaporation Technique

High purity Zn chips was thermally evaporated from molybdenum boat by using Belzar coating unit at vacuum of 10^{-6} mbar on to an other oriented quartz single crystal with following condition:

The required amount of Zn chips was put in a boat mounted under the funnel and between two electrodes in the vacuum chamber. A Quartz substrate was fixed on a spherical holder and placed in position at height of about 5cm above the boat. When the system was pumped down, an electric current was passed through the boat gradually to prevent breaking the boat when the boat temperature reached to the required temperature, the deposition process starts after this step, the current supply was switched off and the samples were left in the vacuum for a day. Then the air was admitted to the chamber and the films were taken out from coating unit to determine the structure of the films.

Results and Discussion

1. Indexing back reflection Laue pattern

Table (1a) shows the input data for Orient Express of quartz crystal taken from powder diffraction file PDF no.(33-1161) while table (1b) shows the (X,Y) coordinates measured from fig. (1a) of the selected spots and the indices (hkl) assigned by orient express to these spots. Figs. (2a&2b) show the simulated patterns of Laue back reflection of quartz marking the indices of the prominent zones. Comparison between the simulated pattern fig. (2b) with the experimental Laue pattern Fig. (1a) indicate correct coincidence of the two patterns an indication to the successful achievement of crystal orientation. It is also found that the quartz crystal is nearly oriented in the [001] direction.

Table 1a: Orient express Input data of quartz crystal.

System Hexa	
a(Į):	4.913
b(Į):	4.913
C(Į):	5.405
α:	90.00
β:	90.00
Ĩ:	120.00
Group:	P-1
Dist(Cm)	3.00
Angle°:	180.00
λ1	0.3000
λ2	3.000
D.Hight (Cm)	11.5
D.Width (Cm)	9.0

Table.1b: Coordinates of selected diffraction spots and their indices (hkl).

No.	X(Cm)	Y(Cm)	h k l
1	2.05	0.60	0 0 -1
2	-1.55	-1.20	-1 1 -2
3	-0.60	-3.70	-2 1 -3
4	2.35	-4.75	-1 0 -2
5	-1.30	2.80	0 1 -2
6	-2.85	4.10	0 3 -5

2. Quartz Crystal as Substrate for Thin Film

Fig.(3a) shows XRD pattern of quartz prior to coating showing sharp single peak of (101) reflection at 2θ =26.7 degrees an indication to the singularity of the quartz crystal. As the quartz crystal is coated by Zn metal film, the XRD shown in fig. (3b) reveal sharp peak at 43.5 degrees correspond-ding to (101) reflection of Zn structure in addition to two very small peaks namely (002) and (100) that are caused by the mosaic structure of the Zn film. In order to evaluate the validity of the singularity of Zn film, a comparison is made with the polycrystalline spectra of Zn PDF no. (4-831) as in table (2). The relative intensities of the (002) and (100) reflections in Zn single crystal film are one order less than for the polycrystalline Zn, a clear indication to the singularity of the deposited Zn film. Moreover, the appearance of the (002) and (100) are thus due to mosaic structure of the Zn film and can then be considered as a single crystal film grown in the [101] which conform with substrate orientation.

Table 2: Relative intensities of single and polycrystalline quartz for three Reflections.

Reflections	2θ degrees	Relative Intensity (%)	
		Polycrystalline	Single Crystal
(002)	36.2	53	3.3
(100)	35.0	40	5.0
(101)	43.5	100	100

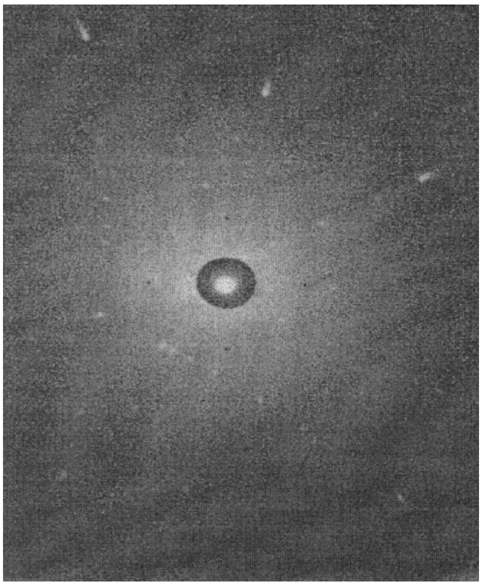

Fig. 1a: Typical back-reflection Laue photograph of Quartz crystal.

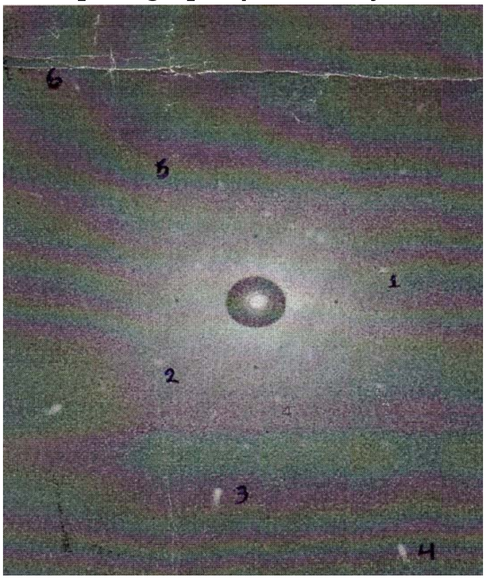

Fig. 1b: Back reflection Laue pattern for Quartz crystal marked with the selected poles of several prominent zones.

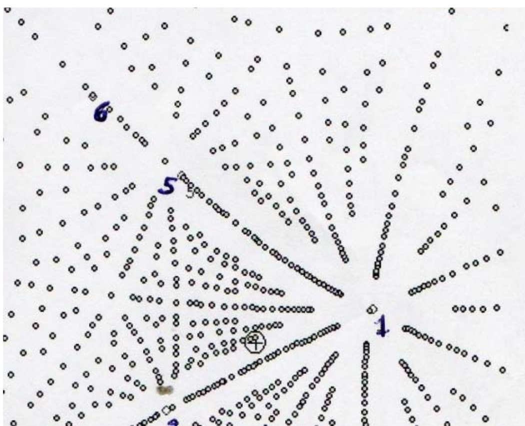

Fig. 2a: Simulated back reflection Laue pattern.

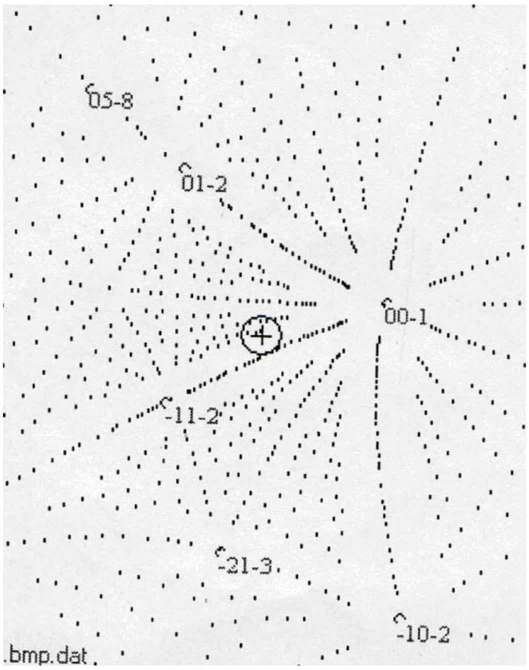

Fig 2b: indices assigned to the simulation in fig. 1a

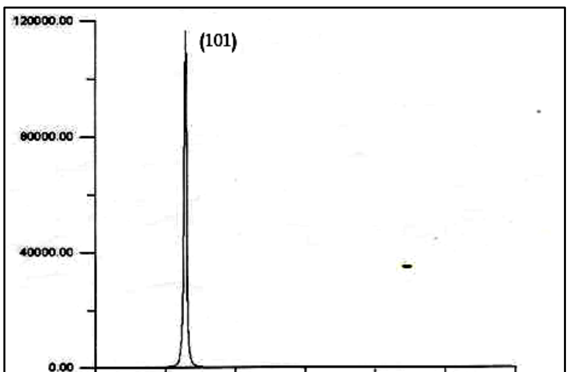

Fig. 3a: XPD pattern of original quartz crystal.

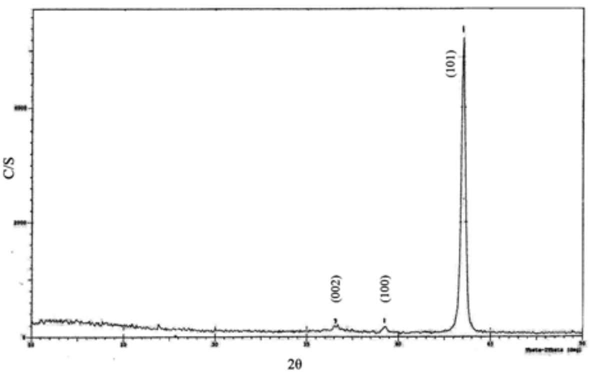

Fig. 3b: XRD pattern of Zn film deposited on quartz crystal

Conclusion

The conclusion drawn from this work is that indexing of Laue back reflection of quartz single crystal can be achieved by the manipulation of Orient Express- program. The singularity of the Zn metal film thermally evaporated on quartz single crystal is governed by the mosaic structure of the grown Zn film and it may be said that better control of evaporation parameters are necessary to minimize the mosaic structure of the Zn film and thus achieve better degree of singularity.

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