Photoluminescence and Photoconductivity Studies of NaBi(WO$_4$)$_2$ Single Crystals: A promising Cherenkov radiator

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Introduction

Single crystal of NaBi(WO$_4$)$_2$ (NBW) is one of the promising materials that can be used as a Cherenkov detector for both luminosity and calorimetric measurements under higher charge backgrounds that are encountered in the high energy physics experiments [1-2]. From the chemical point of view NBW may be regarded as related to PbWO$_4$ (PWO) with the replacement of Pb by a 1:1 mixture of Bi and Na. Optical and luminescent properties of NBW are scarcely studied and it was reported that X-ray luminescence spectrum has a maximum at ~520 nm and the luminescence intensity is about 5% that of Bi$_4$Ge$_3$O$_{12}$ (BGO). However there is no report on photoconductivity properties of this material.

In the present paper we report on spectral dependence of the photoconductivity in conjunction with photoluminescence of NBW crystals and thermal activation energy for its quenching. These are highly desirable parameters for a crystal to be used as a Cherenkov radiator.

Experimental details

The crystals used in the present investigation were grown using the Czochralski technique. Photo-luminescence (PL) studies were performed over a wavelength range from 300 nm to 800 nm and in a temperature range of 77–300K by employing a fluorescence spectrometer (Edinburg Model-FLP920). The emission was recorded in the reflection geometry by positioning the samples at an angle of 45° to the excitation beam. A xenon lamp was used as the excitation source and a spectral bandwidth of 1 nm was selected for both excitation and emission monochromators. A cryostat (Oxford, Optistat-DN) was used for low-temperature measurements. The recorded luminescence spectra were corrected for the spectral sensitivity function of the instrument. The correction file was prepared by recording the spectra under identical conditions replacing the sample by a standard scatterer.

The spectral dependence of photoconductivity was measured at a dc field of about 500 V/cm applied using gold electrodes deposited on one side of the crystal sample. Lock-in amplifier was used to measure the photocurrent.

Results and discussion

The emission spectra recorded for an NBW crystal at 77 K, showed a broad emission band peaking at ~495 nm (Fig.1). The temperature dependence of 495 nm emission is also shown in the inset of Fig.1. The PL intensity becomes half at ~145 K and completely quenched beyond 200K.

Fig. 1 Spectral dependence of emission of NBW crystal.

The observed temperature dependence is also consistent with the reported results for other AWO$_4$-type crystals. The anisotropy in emission band and temperature dependence of emission indicated the presence of more than one excited states. Therefore PL intensity quenches with

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increasing the temperature as non-radiative transitions increase.

Two excitation bands peaking at ~280 nm and 322 nm were observed for the 495 nm emission as shown in Fig.2. A large stoke shift of ~10854 cm⁻¹ for the emission band was found to be similar to other molybdate and tungstates and therefore indicates excitation and emissions to be based on singlet–triplet transitions. Fig.3 shows total and partial density of states of NBW and its constituent atoms as reported recently [3]. It was observed that the valence band (VB) is mainly formed by non-bonding states of the oxygen p orbital, with a very little contribution coming from the tungsten d orbital. The conduction band (CB) is mainly formed from W d states with a similar amount of contributions coming from the p states of bismuth and oxygen. Thus the band gap in the NBW is of charge transfer character involving the (WO₄)²⁻ units similar to other tungstates like PbWO₄.

However, unlike PbWO₄, the photoconductivity lies in the excitation region of NBW crystals where band to band transition is involved. Comparing the spectral dependence of excitation, photoconductivity and transmission of the NBW crystal, only intrinsic photoconductivity could be observed in these crystals. Information regarding excitation and relaxation of excited states are highly desirable to use these crystals as a Cherenkov radiator.

Photoconductivity observed in the excitation region indicates that it yields free charge carriers. Therefore mobile charge carriers are involved in the luminescence and excitation processes in the case of NBW crystals. These processes are corresponding to the delocalized transitions in contrast to the localized transitions in case of PWO. This may be one of the reasons for lesser activation energy of the thermal quenching of photoluminescence in the NBW crystals compared to that for the PWO crystals. This thermal activation energy for the quenching can be calculated from a Mott-Seitz temperature dependence of photoluminescence as shown in Fig.1. This energy for the 495 nm emission was calculated to be about 160 meV in the case of NBW crystals which is smaller than that for PWO (~200 meV). To use these crystals as Cherenkov radiator it is an important parameter making NBW more promising compared to PWO crystals that are deployed currently in the high energy physics experiments at CERN.

References