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# Characterization of electronic structure in dielectric materials by making use of the secondary electron emission

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ABSTRACT

The methodology of characterizing electronic structure in dielectric materials will be presented in detail. Energy distribution of the electrons emitted from dielectric materials by the Auger neutralization of ions is measured and rescaled for Auger self-convolution, which is restructured from the energy distribution of the emitted electrons. The Fourier transform is very effective for obtaining the density of states from the Auger self-convolution. The MgO layer is tested as an example of this new measurement scheme. The density of states in the valence band of the MgO layer is studied by measuring the energy distribution of the emitted electrons for MgO crystal with three different orientations of (111), (100) and (110). The characteristic energy of $\varepsilon_0$ corresponding to the peak density of the states in the band is determined, showing that the (111) orientation has a shallow characteristic energy $\varepsilon_0 = 7.4$ eV, whereas the (110) orientation has a deep characteristic energy $\varepsilon_0 = 9.6$ eV, consistent with the observed coefficient $\gamma$ of the secondary electron emission for MgO crystal. Electronic structure in new functional nano-films spayed over MgO layer is also characterized. It is therefore demonstrated that secondary electron emission by the Auger neutralization of ions is highly instrumental for the determination of the density of states in the valence band of dielectric materials. This method simultaneously determines the valence band structure and the coefficient $\gamma$ of the secondary electron emission, which plays the most important role in the electrical breakdown phenomena.



## 1. Introduction

Various metal oxides have been reinvestigated in an attempt to determine new capabilities of plasma generation, which is the first step in the research and development of semiconductors [1–3], solar cells [4,5], and display [6,7] industries. The material properties of dielectric layers created from these oxides are important when seeking to upgrade the performance of solar cells and display devices. In addition, mixtures of various dielectric materials, including nano-particles, will be used in the future. The key issue in these dielectric layers is the electronic structure in the layer, particularly the valence band, whose detail structure dominates the performance of these devices. For example, the emission time and the amount of secondary electron emission [8–11] from the MgO protective layer in the discharge cells in a plasma display panel (PDP) together play a pivotal role in the electrical discharge and the light emission of a plasma display panel. However, these secondary electron emissions are directly related to the valence band in the MgO layer. It is therefore important to investigate the properties of the valence band structure in dielectric layers. There are various methods [12–22] to determine the band structure of different materials. For example, photoelectron spectroscopy [16] can be used to determine the valence band structure. X-ray photoemission spectra [20–22] and photoluminescence spectral measurements [23] have also been utilized to determine the valence band structure. Particularly, discussion of the interplay between external fields and the work function in secondary electron emission is presented in Ref. [22]. In this context, a new means of measuring the band structure by an ion beam was proposed in a brief report [24]. This article presents a detailed description of measuring the valence band structure in MgO layers by the secondary electron emission from Auger neutralization of ions. This is the first experimental attempt to determine the valence band structure of MgO layer, although the measured data in this article might not necessarily be the most accurate results. Electronic structure in new functional nano-films spayed over MgO layer is also investigated by this new measurement scheme. This method simultaneously determines the valence band structure and the coefficient $\gamma$ of the secondary electron emission, which plays the most important role in the electrical breakdown phenomena.

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Electrons are emitted from a dielectric layer when ions move close to the film surface due to Auger neutralization [25]. Preconditioning of the dielectric film must be carried out before the energy distribution measurement of emitted electrons. The profile of the energy distribution of the emitted electrons can be measured and rescaled so that Auger self-convolution arises, revealing the detail structure of the valence band, including all of the necessary band information. Particularly, the properties of the valence band in MgO layers are investigated here as an example of the determination of the band structure. This can be applied as a relevant technology for PDPs by making use of Auger self-convolution from the measured electron distribution.

A brief discussion of the Auger self-convolution for secondary electron emission is discussed in Section 2, presenting a specific example of obtaining the self-convolution from the energy distribution of emitted electrons. The density of states (DOS) in the valence band may be obtained from the Auger self-convolution determined experimentally. Section 3 presents the Fourier transform for obtaining the DOS from the Auger self-convolution, specifically demonstrating the effectiveness of the transform analytically and numerically. The density of states in the valence band of the MgO layer is discussed in Section 4 after measuring the energy distribution of the electrons emitted from the MgO crystal with three different orientations of (111), (100) and (110). The characteristic energy of $\varepsilon_0$ corresponding to the peak density of the states in the band was determined, showing that the orientation (111) has shallow characteristic energy $\varepsilon_0 = 7.4$ eV, whereas the orientation (110) has a deep characteristic energy $\varepsilon_0 = 9.6$ eV, which is consistent with the observed coefficient $\gamma$ of the secondary electron emission for the MgO crystal. The density of state in the valence band for MgO film and MgO film with a functional layer (FL) deposited over a dielectric surface is investigated in Section 4. The peak of the density function $f_e(\alpha)$ for MgO film occurs at $\alpha = 7.5$ eV for film with an FL and 8.6 eV for film without an FL. The density function $f_e(\alpha)$ for MgO film with an FL is shallower than that for the MgO film without, indicating greater secondary electron emission. Section 4 demonstrates that the secondary electron emission by the Auger neutralization of ions is highly instrumental for determination of the density of states in the valence band of dielectric metal oxides.

## 2. Auger self-convolution of secondary electron emission

A noble gas ion with ionization energy $E_i$ approaches the surface of a dielectric layer, as shown in Fig. 1, where the focused ion-beam system shown in the figure consists of a thermal electron source, the ionization and acceleration region of the ions, a single electrostatic Einzel lens to focus the ion beam, and a collector and copper pad to measure the electron emission from the dielectric layer. The neutral gases released from the mass flow controller are ionized after colliding with the thermal electrons generated from the hot filament. These ions are accelerated by the electric field that forms between the anode and the grounded electrode, and the ions are extracted and accelerated to the downstream region of the electrostatic Einzel lens through a 2 mm diameter hole in a grounded electrode. The ion energies are adjusted by the anode voltages. The ion beam is focused by the single Einzel lens. The electrons are emitted from the dielectric layers due to the Auger neutralization mechanism of the incoming low-energy ions. When the collector potential is strongly negative-biased, the electric field is polarized toward the collector from the grounded copper pad. The electrons emitted from the films by the ion bombardment then come back to the dielectric layer and only the ion current ($I_i$) coming to the film is measured. On the other hand, the positively biased collector orients the electric field toward the grounded

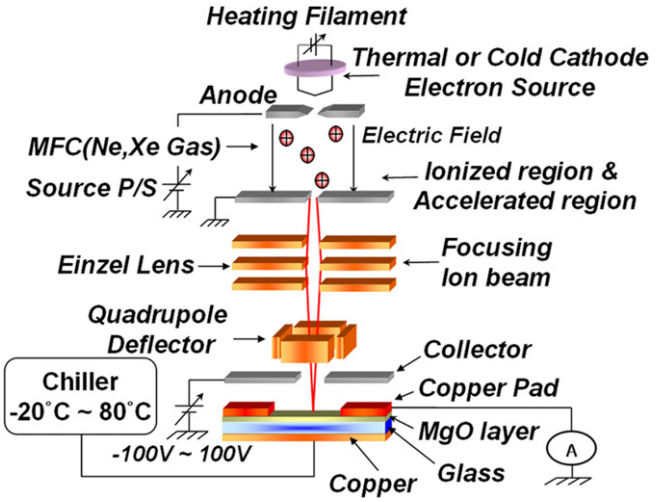


**Fig. 1.** (Color online). Schematic representation of the focused ion-beam system consisting of the thermal electron source, the ionization and acceleration region of the ions, the single electrostatic Einzel lens to focus the ion beam, and the collector and copper pad to measure the electron emission from the dielectric layer. [For interpretation of color referred in this figure legend, the reader is referred to web version of the article.]

copper pad. As a result of this electric field, electrons emitted from the film by the ion beam move to the collector, registering the current ($I_t$) in the ampere meter shown in Fig. 1, including the emitted electron current and the ion beam current. The coefficient $\gamma$ of the secondary electron emission is experimentally determined by $\gamma = (I_t - I_i)/I_i$.

The background pressure of the FIB system was maintained at $1.6 \times 10^{-6}$ Torr. The ion acceleration voltage at the anode varies from 50 to 500 V, of which 150 V was used in this experiment. The accelerated ions bombard surface of the MgO films, emitting secondary electrons. The surface charging [26] of the dielectric films makes the measurement of the secondary electron emission difficult. To avoid the charging-up problem on the MgO film during the electron emission measurement, we must scan the MgO surface by a probe ion beam [27] before the measurement. This scanning process also cleans the MgO surface, establishing the electrical path from the MgO film to an adjacent copper pad due to the radial electric field generated by the focused scanning ion beam [27]. Therefore, the surface charging state of MgO film during the measurement was negligible in the experiment, ensuring the universality of the kinetic energy of emitted electrons. However, this scanning process might create some defects on the surface of MgO layer, resulting in some erroneous signals of electron emission. We therefore carried out the surface cleaning with great care, hoping not to generate any surface defections.

Fig. 2 shows the current signal, represented by the solid squared curve and captured by a picoammeter connected to the grounded copper pad, in which the collector voltage varies from 0 V to +15 V at a dielectric layer temperature of −20 °C. Helium ions with $E_i = 24.58$ eV are used in Fig. 2, and the dielectric layer is an MgO crystal that is 7000 Å in thickness. The electron emission depends on the crystal orientation [28]. The crystal orientation of this measurement is (111). We point out that the solid square curve in Fig. 2 represents the total current contributed by ions and electrons. Particularly, the electron current may represent electron emission due to Auger neutralization, the regular cascade-type secondary electron emission, the hole–hole interaction in Auger, etc. But, the coefficient $\gamma$ of the secondary electron emission due to Auger neutralization defined by