Microstructure Characterization of Er₂O₃ Thin Films by Grazing incidence X-ray Diffraction

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Introduction

With the development of silicon based integrate circuit (IC) technology more and more attention was paid in finding the high-k gate dielectric films that can replace for the traditional thin silicon oxide films. The epitaxial growth of the rare earth (RE) metal oxide films has gained from Si-based industry recently because these films have high dielectric constant, good thermodynamic stability, etc. Erbium oxide (Er_2O_3), with high dielectric constant, wide band gap and relatively large conduction band offset, maybe a promising candidate as suitable gate dielectric layer in complement ary-metal-oxide-semico nductor (CMOS) device materials.

In this investigation, we studied the microstructure characterization of epitaxially grown Er_2O_3 thin films on the Si substrate by using grazing incidence x-ray diffraction (GIXD).

Experimental

Er₂O₃ films were deposited in a multi-chamber Si molecule beam epitaxy (MBE) system with a base pressure of about 3 x 10⁹ Torr, by using a metallic erbium source. 1.5-in. p-type Si(111) and Si(001) wafers with resistivity of 2-10Ωcm were used as substrates. Clean Si(111) and Si(001) surfaces were prepared for the growth of Er₂O₃ films. The clean surfaces were prepared by dipping them in dilute HF solution after cleaned with Shiraki method and then desorping the adsorbed H atoms at high temperatures in vacuum. The growth was carried out at a temperature of 700°C with oxygen partial pressure of about 7 x 10⁶ Torr. Film surface morphologies were obtained using atomic force microscopy (AFM).





Fig. 1: Phi scan from 0 to $\pi(a)$ and longitude scans around each Bragg peaks of thin film grown on the Si(111)

Fig. 1 shows the Phi scan from 0 to π and the longitude scans around each Bragg peaks of sample $\text{Er}_2\text{O}_3(110)$ // Si (111). The results shows that Bragg diffraction occurs in

three crystal planes of $\{220\}$ respectively whose inclinations are all 60°, the erbium thin film is monocrystalline and the orientation relationship is Er_2O_3 (110) // Si (111) and the plane 400 is parallel to the plane 220 of the Si substrate. From fig. 1(b) we can find that the angular differences between the Bragg diffraction peaks of the substrate and the thin film are different which can be concluded that there exists strain in different orientations, and the accurate thickness, density, and roughness were obtained by simulating the experimental reflectivity patterns.



Fig. 2. Results of grazing incidence x-ray diffraction of erbium thin film grown on Si (001) substrate.

Fig. 2 shows the results of grazing incidence x-ray diffraction of erbium sample grown on the Si (001) substrate. Two ordered domains which are vertical each other were found from the results, and two Bragg diffraction peaks occur around the diffraction peak of the Si substrate. Two vertical ordered domain are (-440), (004)(a) and (4-40), (-400)(b). The lattice mismatch Δd and the strain (ϵ), the maximum intensity ratio, FWHM and the ordered-domain sizes can be obtained from the results, by which we can characterize the domain profile accurately. The ordered domain occurred in the erbium thin film grown by MBE is an interesting phenomenon. Our research will afford some instructions in finding the promising candidates for the conventional SiO₂ dielectric material.

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