Contract Lattice Constant in Epitaxial MgO Thin Film from Point View of *ab initio* Calculation

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I. INTRODUCTION

When An X-ray irradiates materials with crystal structure, the X-ray penetrates into the materials and is interfere with atoms which periodically arranged in the materials; crystal. Xray behaves as travelling waves just like ripples just like when you throw a pebble into a pond. When the ripples hit a piling, the reflected ripples will interfere with other reflected ripples at other pilings. Depending on the size and distance of pilings, the reflected ripples overlap and interfere constructively. An X-ray reflects at atoms of crystal structure instead of pilings in a pond, and interferes constructively by periodic structure of single crystal in a microscopic size with a wavelength of a few angstrom. An X-ray also behaves as flash of light. While the reflection of light between two surfaces causes an interfere pattern called Newton's rings, the reflection of X-ray between the film surface and substrate also causes an interfere pattern; X-ray reflection method, so called XRR. As the same as Newton's ring can estimate the thickness between the two surfaces, XRR can evaluate film thickness and surface roughness. In this presentation, we introduce examples of contracted lattice constant in epitaxial magnesium oxide (MgO). The contracted lattice constants were verified by ordinal XRD methods (θ-2θ scan) together with in-plain θ-2θ scan to evaluate crystal structure in-plain directions. In order to explain the reason of the contracted lattice constants, we used two approaches of crystallographic aspect (domain epitaxial growth) and chemical stability (first principles calculation). With domain epitaxial growth [1], the contraction of lattice constant reduced the epitaxial film with coincident site lattice (CSL). [2]. To visualize the domain mismatch the authors proposed CSL polar figure in which coherent strain was depicted on polar coordinates. [3] On the other aspect, by applying the ab initio method , optimal lattice constants were evaluated on MgO structure with variety of defect models. Among variety of point defect models, MgO structure with Schottky defects showed the contracted lattice constants.

II. EXPERIMENTAL

MgO samples were prepared on Si(001) substrates by either of pulsed laser deposition (PLD) or sputtering method. After RCA cleaning on the Si(001) substrate, the thickness of the SiO2 layer on the surface was estimated to be 0.4nm by an ellipsometer, assuming a refractive index of 1.46 for SiO_2. The MgO film was deposited on the Si(001) substrate by (1) rf magnetron sputtering using a magnesium metal target, in a mixture of Ar and O_2 ambient atmosphere [3]