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## Structure of coherent $\text{Mg}_3\text{TiO}_4$ oxide formed between TiN and MgO

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### ABSTRACT

Solid state reaction in nanometer scale at the interface between TiN and MgO can result in formation of  $\text{Mg}_3\text{TiO}_4$  particles which has not reported before. The structure of the newly found oxide is characterized with spherical-aberration corrected scanning transmission electron microscopy at atomic resolution with x-ray energy dispersive spectroscopy. The nanosized  $\text{Mg}_3\text{TiO}_4$  oxide particles formed in MgO underneath the epitaxial TN film with cube-on-cube coherent relationship with both MgO and TiN, i.e.  $\text{TiN}(100) \parallel \text{Mg-Ti-O}(100) \parallel \text{MgO}(100)$  and  $\text{TiN}[110] \parallel \text{Mg-Ti-O}[110] \parallel \text{MgO}[110]$ .  $\text{Mg}_3\text{TiO}_4$  is identified to have cubic structure (lattice parameter  $a = 0.842 \text{ nm}$ ) with space group of  $Fd\bar{3}m$ .

**Keywords:** Interface, particles, structure, electron microscopy

### 1. Introduction

Titanium nitride (TiN) epitaxial film grown on MgO substrate has been studied extensively for understanding the growth kinetics and film properties because a high quality film can be easily obtained as a result of both TiN and MgO having the same cubic rock salt structure (space group  $Fm\bar{3}m$ ) with similar lattice constant ( $a_{\text{TiN}} = 0.424 \text{ nm}$  and  $a_{\text{MgO}} = 0.421 \text{ nm}$ ) [1,2]. Recently, spherical-aberration corrected annular dark field scanning transmission electron microscopy (ADF-STEM) which provides atomic resolution capability has become a powerful and mainstream technique for investigation of interphase and grain boundaries with phase and structural changes as the ADF-STEM image in Z contrast can provide precise and simple interpretation about the atomic structure in details [3-5]. In our previous study of the TiN/MgO interfacial structure by applying STEM, positions of atomic columns for Ti, Mg, O, and N can be revealed at atomic resolution from which a fully coherent diffuse interface between TiN and MgO can be recognized [6]. The interdiffusion between TiN and MgO may result in further formation of

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