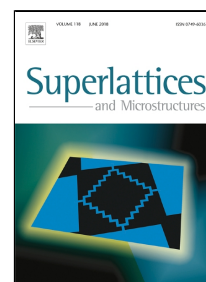


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## Transition of dominant lattice sites of Mg in InN:Mg revealed by Raman scattering

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**Abstract:** The behavior of Mg dopants in InN films grown by molecular beam epitaxy was studied by Raman scattering in a wide Mg concentration ( $[Mg]$ ) range from  $1 \times 10^{16}$  to  $4 \times 10^{21}$  cm<sup>-3</sup>. Transition of dominant lattice sites of Mg dopants was investigated through a diffusion-collision model based on Mg-related local vibrational modes, which was further confirmed through stress analysis. It was found that Mg<sub>i</sub> and Mg<sub>In</sub>-N-In<sub>i</sub> are the dominant sites of Mg dopants at  $[Mg] < 1.8 \times 10^{20}$  cm<sup>-3</sup>, while the complex of Mg<sub>In</sub>-N-Mg<sub>i</sub> dominates with further increasing  $[Mg]$ . This study provides an insight on the behavior of Mg and would be helpful for achieving effective p-type doping in InN.

**Key Words:** Mg-doped InN; Molecular Beam Epitaxy; Raman scattering; Local vibrational modes

### 1. Introduction

As a member of III-nitrides, InN has become more attractive after finding its bandgap being as narrow as 0.64 eV at room temperature [1-6]. This narrow bandgap makes it possible to fabricate III-nitrides-based devices such as laser diodes at optical communication wavelength, high efficiency tandem-structure solar cells and so on [7-13]. One crucial step to fabricate these devices is the p-type doping of InN, which has been attempted by several groups using Mg as the dopant [14-18]. However, the understanding on the doping effect/behavior is not yet enough and a thorough investigation of Mg-doped InN by various techniques is still necessary [19-21].

Raman scattering spectroscopy is a powerful tool for assessing residual strain, crystalline quality and defect structure. It has also been widely used for studying Mg-doped GaN, where the strain-induced defects and local vibrational modes (LVMs) such as Mg-H complexes have been observed [22,23]. In particular, some LVMs have been reported to show evidence of being related to p-type conduction. In comparison, the Raman scattering study on InN:Mg is much less, in particular the Mg-related LVMs mode [24-27].

In this letter, doping behavior of Mg in InN films grown by molecular beam epitaxy (MBE) was investigated in details by Raman scattering in a wide Mg concentration ( $[Mg]$ ) range. Transition of dominant lattice sites of Mg dopants was investigated through a diffusion-collision model based on Mg-related local vibrational modes, which was further confirmed through stress analysis. This study provides an insight on the behavior of Mg and would be helpful for achieving effective p-type doping in InN.

### 2. Sample Fabrication and characterization

A series of InN films with varied  $[Mg]$  were grown on Ga-polar GaN/c-Al<sub>2</sub>O<sub>3</sub> templates by MBE. The Ga-polar GaN/c-Al<sub>2</sub>O<sub>3</sub> templates were grown by metal-organic chemical vapor deposition (MOCVD). After depositing an 80-nm-thick GaN layer, a 50-nm-thick undoped InN layer and a 400-nm-thick InN:Mg layer were

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