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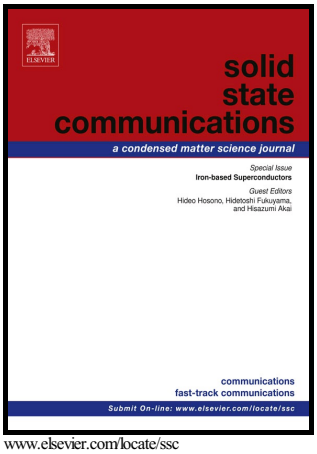

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Formation of Mn-Si$_n$ complexes in GaN: a first principles investigation

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Abstract

Using first principles calculations, we study the relative spatial distribution of Mn and Si impurities in the host matrix of GaN. It stems from our investigation that the co-doping of (Ga,Mn)N with Si will result in the formation of Mn-Si complexes with a large absolute pairing energy of 2.27 eV. The formation of such complexes is energetically feasible already at the growth surface. According to our results, larger complexes involving two Si ions are also possible in bulk but exhibit a much smaller absolute pairing energy. Finally, the co-doping of (Ga,Mn)N with Si results in the reduction of the charge state of Mn from 3+ to 2+ regardless of the relative position of Si and Mn in the gallium sublattice.

Keywords: first principles calculations, gallium nitride, manganese, silicon

1. Introduction

Nitride semiconductors doped with transition metals (TMs) are more challenging materials for growth and characterization than their III-V counterparts. Mn-doped GaN is not the exception. One of the problems in the growth of Mn-doped GaN is the presence of multiple charge states of Mn and their spatial distribution. When the TM doping concentration exceeds the solubility limit for the particular ion in GaN, there is a strong driving force for the TM ions to cluster [1]. As a result, there are regions of high and low TM concentrations.

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