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Stability of Mg-incorporated InN surfaces: first-principles study¹ T. AKIYAMA, K. NAKAMURA, T. ITO, Mie Univ., Japan, J. -H. SONG, A. J. FREEMAN, Northwestern Univ. — InN films are attractive materials for electronic and optelectronic applications. The growth of InN eptitaxial films with *n*-type and *p*-type conductivity has traditionally been performed along the polar <0001> direction², which may result in large polarization fields along the growth direction, reducing the radiative efficiency of quantum-well light emitters. To overcome this drawback, the growth along nonpolar orientation such as (1010) and (1120) planes and its *p*-type doping have been recently carried out. We have addressed this issue by performing first-principles pseudopotential calculations for Mg-incorporated InN surfaces in various orientations, including (1010) and (1120) as well as (0001) and (0001) surfaces³. The calculated surface energies demonstrate that qualitative trends in the stability of Mg-incorporated surfaces agree with those on GaN surfaces ⁴, although several surface reconstructions different from those on GaN surfaces are obtained. The effects of growth conditions on *p*-type doping are also discussed.

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