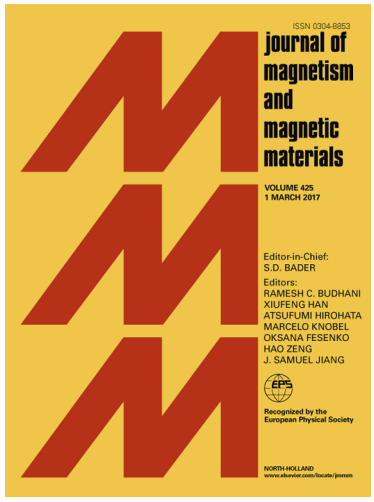

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Boron, nitrogen, and nickel impurities in GeC nanoribbons: a first-principles investigation

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Abstract

Using first-principles calculations based on the density functional theory we investigated the structural, electronic and magnetic properties of substitutional boron, nitrogen, and nickel impurities in germanium carbide (GeC) nanoribbons. Hydrogen terminated GeC ribbons with armchair and zigzag edges are considered here. We observed that all three impurities preferentially substitutes the Ge atom at the ribbon edge. In addition, the electronic band structures of the doped systems indicate that (i) the impurities could introduce impurity bands in the band gap and resulting in a reduction of the band gap of 7-AGeCNR, (ii) the metallic behavior of 4-ZGeCNR turns into semiconductor because of the incorporation of the impurities, (iii) the impurities could change the magnetic moment of 4-ZGeCNR and even introduce magnetic moment into the non-magnetic 7-AGeCNR.

Key words: Density-functional theory; germanium carbide nanoribbons; Boron, nitrogen, and nickel; magnetic moment