Manifestation of the Kirkendall effect in the process of thermal decomposition of $In_xGa_{1-x}N$/GaN MQWs – first principles studies

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In the last decade InGaN/GaN multi-quantum wells (MQWs) applied in light-emitting diodes (LEDs) and laser diodes (LD) have found many applications in illumination technology, medicine, or environmental protection. It is well known that the structural quality of the active regions $In_xGa_{1-x}N$/GaN, that is, the compositional homogeneity of multiple QWs (MQWs), as well as their interfacial morphology, has a significant impact on device performance. As reported by several authors e.g. [1], In-rich InGaN QWs tend to degrade during the growth of p-type capping layers, which reduces the optical properties of the InGaN QW active region. This phenomenon has been observed in both single and MQW structures $In_xGa_{1-x}N$/GaN [2,3]. Recently we have shown that the Kirkendall effect can be the mechanism responsible for the thermal decomposition of the $In_xGa_{1-x}N$/GaN MQWs structures due to triggering of the unbalanced diffusion fluxes of the In and Ga atoms throughout the $In_xGa_{1-x}N$/GaN interface and the formation of voids [4]. Our studies were limited to the description of diffusion process of neutral point defects, that is, Ga, In, and N vacancies.

In this paper, we discuss the diffusion of both neutral and charged point defects across the $In_xGa_{1-x}N$/GaN interfaces based on first-principles calculations. By applying harmonic transition state theory, nudged elastic band method, and phonon calculations, we determined the heights of the migration energy barriers of both neutral and charged metal vacancies diffusing in $In_xGa_{1-x}N$ alloys (x=0, 0.11, 0.22), the vibrational frequencies of $In_xGa_{1-x}N$ alloys in the presence of migrating point defects, and the temperature dependencies of the defect migration energy barriers. We took into account values of the formation energies and concentrations of point defects as a function of temperature, which allowed us to determine the diffusion coefficients of Ga and In atoms migrating in $In_xGa_{1-x}N$ alloys. We showed that the diffusion of charged metal vacancies was more crucial than that of neutral ones in the studied systems, and it contributed the most to the thermal decomposition of $In_xGa_{1-x}N$/GaN MQWs by triggering the formation of voids in the interface area.

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