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Quaternary $Ga_{1-x}In_xP_{1-y}N_y$ alloys described by clustering of In and N in GaP[1] KOUSHIK BISWAS, ALBERTO FRANCESCHETTI, STEPHAN LANY, National Renewable Energy Laboratory, Golden, CO — The interactions between the different atomic constituents in an alloy affect the microstructure, and ultimately, the electronic properties of the alloy. Specifically, in group III-V alloys the energy of formation of single defects and the binding energy of defect complexes play an important role in determining the microstructure. We present a model that starts from the dilute defect picture and extends to alloys of low to moderate concentrations. Using a valence-force-field (VFF) method we calculate the energy of formation of isolated N and In defects and that of small defect clusters formed by N and In in a GaP host. Considering a 1:2.12 N to In ratio that conserves lattice matching to GaP, we show that in a N concentration range up to $\sim 15\%$, the formation energy of the random alloy can be described by the random probability to form such defect clusters. This approach allows the thermodynamic modeling of the microstructure of quaternary alloys, such as GaInNP, without intricate lattice-energy expansions and Monte-Carlo simulation techniques. In GaInNP, we find that short range ordering due to large atom to small atom preferential binding (i.e. InN+GaP) strongly reduces the energy compared to the random distribution.

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