Practical doping principles

Alex Zunger

Citation: Applied Physics Letters 83, 57 (2003); doi: 10.1063/1.1584074

View online: http://dx.doi.org/10.1063/1.1584074

View Table of Contents: http://scitation.aip.org/content/aip/journal/apl/83/1?ver=pdfcov

Published by the AIP Publishing

Articles you may be interested in

First-principles theoretical analysis of transition-metal doping of ZnSe quantum dots

J. Appl. Phys. 112, 024301 (2012); 10.1063/1.4734841

Tuning the electronic and magnetic properties of carbon-doped ZnO nanosheets: First-principles prediction

J. Appl. Phys. 111, 044329 (2012); 10.1063/1.3688233

First-principles study of Be doped CuAIS 2 for p-type transparent conductive materials

J. Appl. Phys. 109

Practical doping principles

Alex Zunger^{a)}
National Renewable Energy Laboratory, Golden, Colorado 80401
(Received 27 January 2003; accepted 21 April 2003)

with killer defects, or prevent E_F from moving." An example is the use of H during Mg doping 12 of GaN: without H, excessive p-type Mg doping will lead to the spontaneous formation of V_N once the Fermi energy moves sufficiently towards the VBM. But since H acts as a donor, it prevents the movement of E_F towards the VBM, thus defeats the formation of the V_N killer defect. Subsequently, H is annealed out. This rule suggests, for example, that p-type doping of oxides can be facilitated by creating internal oxygen precipitates that eliminate oxygen vacancies, e.g., using NO or NO₂ sources $^{3.5}$ for nitrogen-doping of ZnO, or using Li₂O sources for Li doping of MgO (Ref. 23).

(ii) Doping rules pertaining to chemical potential effects. In general, the second term of Eq. (1) shows how ΔH for formation of anionic or cationic dopants can be regulated via control of the chemical potentials during growth [Fig. 1(b)]. This figure illustrates the fact that the enthalpy of forming