Ion relaxation and hydrogen LVM in H-irradiated GaAsN

Mao-Hua Du[a,*], Sukit Limpijumnong[a,b], S.B. Zhang[a]

[a]*National Renewable Energy Laboratory, Golden, Colorado 80401, USA*
[b]*National Synchrotron Research Center and School of Physics, Suranaree University of Technology, Nakhon Ratchasima, Thailand*

Abstract

First-principles calculations show that the hydrogen configurations in GaAsN depend on how hydrogen is introduced into the sample. Since proton and neutral H have different ground states, the proton injected into the sample by H-irradiation follows a unique energy pathway to form a charged dihydride, instead of the charge-neutral H_2^* monohydride. The subsequent charge neutralization causes the spontaneous canting of the dihydrides. The resulting canted N–2H structure explains the recent puzzling IR observation, the recoveries of the GaAs band gap and lattice parameter, and the dihydride symmetry determined by the XANES experiment. It may also have broad implications for ion implantation studies in other solids.

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