www.elsevier.com/locate/jcrysgro

Density functional theory study of dopant effect on formation energy of intrinsic point defects in germanium crystals

S. Yamaoka, K. Kobayashi, K. Sueoka, J. Vanhellemont

PII: S0022-0248(16)30783-7
DOI: http://dx.doi.org/10.1016/j.jcrysgro.2016.11.072
Reference: CRYS23800

To appear in: *Journal of Crystal Growth*

Cite this article as: S. Yamaoka, K. Kobayashi, K. Sueoka and J. Vanhellemont, Density functional theory study of dopant effect on formation energy of intrinsic point defects in germanium crystals, *Journal of Crystal Growth*, http://dx.doi.org/10.1016/j.jcrysgro.2016.11.072

Density functional theory study of dopant effect on formation energy of intrinsic point defects in germanium crystals

S. Yamaoka[a], K. Kobayashi[a], K. Sueoka[a,*], and J. Vanhellemont[b]

[a] Department of Communication Engineering, Okayama Prefectural University, 111 Kuboki, Soja, Okayama 719-1197, Japan

[b] Department of Solid State Sciences, Ghent University, Krijgslaan 281 S1, Gent B-9000, Belgium

*Corresponding author.

E-mail address: sueoka@c.oka-pu.ac.jp

Abstract

During the last decade the use of single crystal germanium (Ge) layers and structures in combination with silicon (Si) substrates has led to a revival of defect research on Ge. Ge is used because of the much higher carrier mobility compared to Si, allowing to design devices operating at much higher frequencies. A major issue for the use of Ge single crystal wafers is the fact that all Czochralski-grown Ge (CZ-Ge) crystals are vacancy-rich and contain vacancy clusters that are much larger than the ones in Si. In contrast to Si, control of intrinsic point defect concentrations has not yet been realized at the same level in Ge crystals due to the lack of experimental data especially on dopant effects. In this study, we have evaluated with density functional theory (DFT) calculations the dopant effect on the formation energy (E_f) of the uncharged vacancy