

Density functional treatment of extended interstitial defects in Si

R. Jones, T. A. G. Eberlein,

School of Physics, University of Exeter, Exeter EX4 4QL, U.K

J. P. Goss P. R. Briddon

School of Natural Science, Newcastle upon Tyne NE1 7RU, U.K.

A. T. Blumenau

Theoretische Physik, Universität Paderborn, 33098 Paderborn, Germany

S. Öberg

Department of Mathematics, Luleå University of Technology, SE-97187 Luleå, Sweden

Self-interstitials in silicon, produced by ion-implantation or oxygen precipitation, can aggregate to form extended rod-like-defects (RLDs) with unusual $\{113\}$ habit planes and having both electrical and optical activity. Although known for over 30 years they remain an enigma. Here, we describe the results of local density functional calculations on the RLDs which reveal their structure and electrical activity. We find that small $\{113\}$ RLDs are more stable than RLDs condensing onto $\{111\}$ planes but this reverses for larger defects. We attribute the electrical activity of $\{113\}$ RLDs to the bounding dislocations and a pronounced and sharp photoluminescence band to vacant interstitial sites on the RLD. The results of the modelling demonstrate that complex arrangements of interstitials are amenable to theoretical analysis and give hope that the pathways to other extended defects can also be found.