E centers in ternary Si$_{1-x-y}$Ge$_x$Sn$_y$ random alloys

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Si$_{1-x-y}$Ge$_x$Sn$_y$ binary and ternary alloys are considered as highly promising materials for laser, detector, photovoltaic, and microelectronic applications. For example, Ga$_{1-x}$In$_x$As$_y$ quantum wells have been fabricated on lattice matched Ge$_{1-x}$Sn$_x$ buffer layers. Recently, Bauer et al. have managed to synthesize single-phase monocrystalline Si$_{1-x}$Ge$_x$Sn$_y$ alloys with a Si content of up to 32% and a Sn content of up to 10%. In these alloys, the three elements occupy random substitutional sites on the underlying diamond lattice. Notably, in quantum well cells based on GaInP/GaAs/Ge three stack layers, there is a concern over the issue of arsenic penetrating into Ge and effectively doping it. It is predicted that the nearest-neighbor environment will exert a strong influence on the stability of $E$ centers in ternary Si$_{1-x}$Ge$_x$Sn$_y$. © 2009 American Institute of Physics.
The lattice parameters of binary and ternary random alloys can deviate from Vegard’s Law. This means that the lattice parameter of the alloy deviates from the linear interpolation of the lattice parameters of the constituent elements. For $Si_{1-x}Ge_xSn_y$, the deviation from linearity, $\Delta \alpha(x,y)$, is given by

$$\Delta \alpha(x,y) = (1-x-y)\alpha_{Si} + x\alpha_{Ge} + y\alpha_{Sn} - \alpha_{SiGeSn},$$

(1)

where $\alpha_{Si}$, $\alpha_{Ge}$, $\alpha_{Ge}$, and $\alpha_{SiGeSn}$ are the lattice parameters of Si, Ge, Sn, and $Si_{1-y}Ge_ySn_y$, respectively. Therefore, a negative value of $\Delta \alpha(x,y)$ corresponds to a positive bowing of the lattice parameter. As has been determined experimentally by Kouvetakis et al. and reaffirmed using the SQS approach, the bowing of the lattice parameter is negative for $Si_{1-x}Ge_x$, and positive for $Sn_{1-y}Ge_x$. For the $Si_{0.375}Ge_{0.5}Sn_{0.125}$ alloy, we predict a positive bowing of the lattice parameter ($\Delta \alpha = -0.011 \text{ Å}$). This is consistent with previous work for $Si_{1-x}Ge_xSn_y$ in which $\Delta \alpha$ is zero when the Sn:Si content ratio is 0.333. Since we have considered an Sn:Si content ratio of 0.333, the lattice parameter should have a positive bowing as predicted.

$Si_{1-x}yGe_xSn_y$ is a random diamond structure alloy in which Si, Ge, and Sn randomly occupy the same lattice site. As a consequence of the random distribution, the local substitution of an As atom or the formation of a vacancy will occur with a multitude of distinct local arrangements of the surrounding host atoms that will, in turn, affect the energy of the defect. The attraction between As atoms and vacancies can be quantified by calculating the binding energies. For example, the binding energy of an $As_{Ge}$ (that is an As atom at a Ge substitutional site) to a $Sn$ (that is a vacant Sn site) in an $N$ lattice site supercell of composition $Si_{N-x-y}Ge_xSn_y$ is given by

$$E_{b}(As_{Ge}V_{Sn}Si_{N-x-y}Ge_xSn_{y-1}) = E(As_{Ge}V_{Sn}Si_{N-x-y}Ge_xSn_{y-1}) - E(As_{Ge}Si_{N-x-y}Ge_xSn_{y}) - E(V_{Sn}Si_{N-x-y}Ge_xSn_{y-1}) + E(Si_{N-x-y}Ge_xSn_y),$$

(2)

The only exception is $As_{Sn}V_{Sn}$ for which the $V$ is surrounded by three Si atoms. Given the limited size of the SQS cell, it might be prudent in the future to consider a larger SQS cell and further challenge this observation.
prediction of both Ge and Sn atoms at NN sites to the V in Si$_{0.375}$Ge$_{0.5}$Sn$_{0.125}$ is analogous to previous work in Si$_{1-x}$Ge$_x$. In particular, the positron annihilation work of Sihto et al. determined that there is an energy gain when a Ge atom replaces a Si atom next to a V in Si$_{1-x}$Ge$_x$. This experimental observation was also supported by DFT studies using the SQS approach.

The second-NN (2NN) environment around the E center can also affect its stability to a lesser degree compared to the NN environment, but still to a significant extent. For example, the binding energy of an As$_V$Si$_{1-x}$ pair, in which both the As and the V have two Ge atoms and one Si atom at NN sites, can vary as much as 0.34 eV depending on the 2NN environment. This fact is in agreement with previous studies of Si$_{1-x}$Ge$_x$, where the 2NN environment affected the stability of E centers by up to 0.17 eV and the formation of vacancies by 0.10 eV.

The significant impact of the local environment on the stability of the E centers will result in an inhomogeneous distribution of E centers in Si$_{1-x}$Ge$_x$ ternary alloys. Nevertheless, the binding energies of the most strongly bound AsV$_x$ pairs in Si$_{0.375}$Ge$_{0.5}$Sn$_{0.125}$ are within the range of the binding energies of AsV$_x$ pairs in Si (−1.23 eV) and Ge (−0.52). The diffusion properties of the AsV$_x$ pair are also expected to vary with the local changes of composition within the Si$_{1-x}$Ge$_x$Sn$_x$ alloy.

Finally, we only report the lowest energy configurations for which the binding energies were negative. As mentioned before, however, it was predicted that AsV$_x$ pairs can also have positive binding energies depending on the 1NN environment. This would imply that, in specific compositional and configurational regions of the Si$_{1-x}$Ge$_x$Sn$_x$ alloy, the migrating AsV$_x$ pair will be more likely to dissociate into an immobile As atom and a migrating V. In Si$_{1-x}$Ge$_x$, Han et al. predicted, using molecular dynamics, that compositional variations affect the self-diffusion via vacancies. In turn, self-diffusion is deemed to be important for the formation of E centers, with vacancy diffusion being faster in Ge than Si.

In conclusion, electronic structure calculations in conjunction with the SQS approach have been used to study the stability of AsV$_x$ pairs in Si$_{0.375}$Ge$_{0.5}$Sn$_{0.125}$. It was found that AsV$_x$ pairs are more strongly bound in Si$_{0.375}$Ge$_{0.5}$Sn$_{0.125}$ than in Ge alone but less strongly than in Si alone. In Si$_{0.375}$Ge$_{0.5}$Sn$_{0.125}$, the NN environment has a significant impact on the binding energy of the E centers, whereas the effect of the 2NN environment, while significant, is rather smaller.

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