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Defect reaction network in Si-doped InAs: Numerical predictions

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Defect reaction network in Si-doped InAs: Numerical predictions

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Abstract

This Report characterizes the defects in the defect reaction network in silicon-doped, *n*-type InAs predicted with first principles density functional theory. The reaction network is deduced by following exothermic defect reactions starting with the initially mobile interstitial defects reacting with common displacement damage defects in Si-doped InAs, until culminating in immobile reaction products. The defect reactions and reaction energies are tabulated, along with the properties of all the silicon-related defects in the reaction network. This Report serves to extend the results for the properties of intrinsic defects in bulk InAs as collated in SAND 2013-2477: "Simple intrinsic defects in InAs: Numerical predictions" to include Si-containing simple defects likely to be present in a radiation-induced defect reaction sequence.

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TABLES

NOMENCLATURE

CBE	conduction band edge
DFT	density functional theory
eV	electron Volt
FDSM	finite defect supercell model
GGA	generalized gradient approximation
LDA	local density approximation
n/x	not exist
PBE	Perdew/Burke/Ernzerhof, a “flavor” of GGA
PP	pseudopotential
VBE	valence band edge

1. INTRODUCTION

The defect reaction network, the chain of reactions driven by species mobilized in primary displacement damage, is predicted and numerically characterized using first-principles density functional theory for irradiated silicon-doped, *n*-type indium arsenide, InAs. The reaction network is deduced from first principles: identifying the primary defect species likely mobilized during displacement damage, the indium and arsenic interstitials, systematically investigating their reactions with the silicon dopant atom and immobile primary displacement damage defects and inserting into the network those reactions that are exothermic, and following this chain of reactions and incorporating potentially new mobile reaction products until culminating in immobile defects. The numerical predictions associated with this first-principles reaction network are presented in a series of numerical Tables containing parameters to populate a defect physics package needed for device simulations, extending the defect physics parameters predicted for simple intrinsic defects in InAs [1].

Studying the Si reaction network in the binary InAs is more motivated by the need to understand silicon defect behavior in ternaries such as $In_xGa_{(1-x)}As$ rather than defect behavior in the simple binary. Previously, a similar reaction network had been developed from first principles density functional theory for Si-doped (*n*-type) GaAs [2,3]. The simple binary semiconductors are conceptually and computationally simpler to study than a ternary, and the expectation and hope is that the behavior of the radiation-induced silicon reaction network in the intermediate ternary alloys can be understood more readily as intermediate between the silicon reaction networks in the end-member binary compounds. The In and Ga atoms are roughly the same size in the lattice, and have similar chemistries, and similarities in the GaAs and InAs reaction network defects would suggest that the intermediate ternary alloys would exhibit similar behavior, in an atomistic variant of a Vegard's Rule. The predictions in this Report concerning defects in Si-doped InAs indeed bear great similarity to Si-based defects in GaAs, vindicating this hypothesis.

This Report focuses on silicon-containing defects in InAs. Numerical results for density functional theory (DFT) calculations of properties of simple intrinsic defects in indium arsenide have been presented in a previous SAND Report: 2013-2477, "Simple intrinsic defects in InAs: Numerical predictions" [1]. That Report contains detailed Tables of intrinsic defect properties—charge transition defect level energies, formation energies, diffusion barriers—predicted with asymptotically converged DFT. The current report presents the results of DFT calculations for the same defect properties, for silicon-containing defects likely to be present in a defect reaction network instigated by a radiation event. Assessment of defect reaction network energies involving intrinsic defects use values presented in the earlier Report [1].

This Report focuses on first order reactions. Second order or greater (interstitial-interstitial, or interstitial-product) reactions are much less numerous and unlikely to significantly affect the electrical response of the bulk material, these reactions, as in the previous Report on Si-doped GaAs [2,3], are therefore (mostly) neglected. Similarly, because *n*-type silicon doping will preferentially populate defects in their most negative charge states, emphasis is on careful characterization of defect evolution consistent with a Fermi level near the conduction band edge (although all potentially accessible charge states for each defect in the network are examined).

1.1. Computational methods

The details of the computational methods are the same as comprehensively described previously [1], and will only be summarized here.

The DFT calculations are performed with the SEQQUEST code [4], using both the local density approximation (LDA) [5] and the Perdew-Burke-Ernzerhof (PBE) flavor of the generalized gradient approximation [6]. The comparison of LDA and PBE results is a partial assessment of the physical uncertainties inherent with using approximate DFT functionals [7]. The calculations are not spin-polarized; previous results in GaAs indicate the that spin polarization can lower defect formation energies by ~50 meV[13], a relatively modest change less than the physical uncertainties associated with using DFT functionals. The calculations could repeated with spin-polarization to refine these predictions. The pseudopotentials (PP) for In and As are norm-conserving Hamann type [8], and are the same PP used for intrinsic defects calculations [1] and carefully verified. The close correspondence between the 3*d*-core and 3*d*-valence PP for the indium atom are evidence for a good transferability of the 3*d*-core PP for In. Calculations for silicon-containing InAs defects are all done with 3*d*-core pseudopotentials (total valence charge Z=3) for the In atom, and not repeated with 3*d*-valence (Z=13) PP. We had previously determined that the PP construction for the In atom, the 3*d*-core vs. 3*d*-valence, has only modest effect on computed defect properties, the physical uncertainties in the DFT results being dominated by the difference between the physical approximations of LDA and PBE [1]. If deemed necessary, the current calculations could be straightforwardly repeated using the more rigorous 3*d*-core PP for In. The silicon PP in this work are the same used and extensively validated in previous work for defects in bulk silicon [9] and silicon defects in GaAs [2,3]: generalized norm-conserving Hamann potentials [6], with a double-zeta plus polarization contracted-Gaussian basis set, as taken from the SEQQUEST library of optimized, transferable atomic potentials [4].

As previously [1], defect formation energies are quoted in the arsenic-rich limit. The chemical potential of the arsenic atom is set to the computed energy of the arsenic in the elemental bulk ground state *A7* structure, and the chemical potential of the indium atom is set to be that required to make the formation energy of perfect crystalline InAs equal to zero. The chemical potential of a silicon atom is arbitrary, all reactions considered in this Report are silicon number conserving. Here, it is set to the computed standard state of silicon, i.e., the energy of one atom in the crystalline diamond structure of silicon.

The calculations of charged defects use the Finite Defect Supercell Model (FDSM) [9] to incorporate rigorous boundary conditions for the solution of the electrostatic potential in a charged supercell [10,11] and extrapolate the computed defect energies to the infinitely dilute limit. Results for silicon-related defects are presented for 216-site cubic supercells, extrapolated to infinitely dilute limits using the FDSM. Cell-size convergence tests for intrinsic defects using results extrapolated from selected 64-site, 512-site, and 1000-site cubic supercells verify that results using 216-site supercell are numerically well converged [1], to less than the physical uncertainties embodied in the functional, satisfying a key criterion of verification and validation of subcontinuum-scale simulations [12]. The simulation contexts presented here correspond to the “LDA” and “PBE” simulation contexts defined in the Report for intrinsic defects in InAs [1].

1.2. Verification and validation

The silicon-related defect level calculations all use SEQQUEST and the FDSM, the same methods used in DFT calculations of defects in silicon [9], intrinsic defects in GaAs [13,14], and for silicon-related defect chemistry in GaAs [2,3], which yielded mean absolute errors of 0.1 eV and maximum absolute error of 0.2 eV for defect levels over a wide sampling of different defects in bulk silicon [9] and GaAs [13]. This is the expected accuracy (uncertainties) of the methods for defect level calculations in InAs, and is the limit (best possible) of the physical accuracy of the DFT approximations used in this analysis.

Using the same methods and models, the verification and validation of the PP and extrapolation model inherit directly from earlier results for intrinsic defects in InAs [1] and GaAs [13,14].

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2. RESULTS

The section contains the Tables that summarize the numerical results for DFT simulations of silicon-related defects and the radiation-induced defect reaction network in InAs.

The process by which the reaction network is deduced is iterative. It starts with the defects species generated by displacement damage (vacancies and interstitials). Using DFT calculations, we had identified that the self-interstitials in III-V materials are likely to be the mobile species [1,13]. Their reactions with all common immobile defects are investigated, and exothermic defect reactions are added to the reaction network. The "common" immobile defects are the vacancies and the divacancy, being primary displacement damage defects, and the silicon substitutional (dopant) atoms. Reactions between mobile species, i.e., second order reactions, are mostly neglected. One of the reaction products in the reaction network for Si-doped InAs is the silicon interstitial Si_i, and the current results indicate Si_i might also be a mobile specie, just as in GaAs [13,14]. Hence, its reactions with immobile defects are investigated, and the exothermic reaction products are added to the defect reaction network. The same set of defects analogous to the silicon chemistry in GaAs proved relevant in InAs as well. No other reaction products are identified that are likely to be mobile.

2.1. Defect atomic structures

The following Table summarizes the ground state structures for the silicon-containing defects within the defect reaction network. The intrinsic defect structures have been presented previously [1,11] and the same nomenclature is used to describe silicon defect structures as used in the InAs and GaAs intrinsic defects and illustrated for GaAs defects in Ref. 13.

Table 1. Ground state structure description for silicon reaction network defects.

Charge state	Si_{In}	Si_{As}	Si_i	$(Si_2)_{In}$	$(AsSi)_{In}$	Si_{vv}
(2-)	-	-	-	C_2 twist-110_{In}	-	C_{1h} Si_{In}–In_{As}–v_{In}
(1-)	-	T_d	-	C_1 – twice-pucker 001_{In}	-	lda: C_{1h} Si_{In}–In_{As}–v_{In} pbe: C_{1h} v_{As}-Si_{In} paired In-In
(0)	$\{T_d\}^a$	$\{T_d\}^a$	C_{1h} split-001_{As} pucker-As	C_{1h} Si_{In}— bridge-Si$[T_{i,In}]$	C_{1h} Si_{In}— bridge-As$[T_{i,As}]$	C_{1h} v_{As}-Si_{In} paired In-In
(1+)	T_d	-	lda: C_{3v} $Si_i[T_{i,In}]$ pbe: C_{1h} Si_{In}— bridge-In$[T_{i,As}]$	C_{2v} Si_{In} – $Si_i[T_{i,As}]$	C_{1h} Si_{In}— bridge-As$[T_{i,As}]$	C_{1h} v_{As}-Si_{In} paired In-In
(2+)	-	-	$T_{i,As}$	C_{2v} Si_{In} – $Si_i[T_{i,As}]$	lda: C_{1h} Si_{In}— bridge-As$[T_{i,In}]$ pbe: C_{1h} split-001_{In} pucker-As	C_{3v} v_{As}-Si_{In}

(a) The DFT result is not a defect state, but the state is in reality likely a shallow donor (Si_{In}) or shallow acceptor (Si_P), and its level will be *assumed* to be at the respective band edge.

2.2. Defect charge transition energy levels

This section presents the defect charge transition levels of the silicon reaction network defects in InAs, in eV, along with the neutral defect formation energies. The defect level predictions are the fundamental result of this Report, the later formation energies and reaction energies are all derived from these results. The quoted defect levels are thermodynamic values, without regard for whether a kinetic barrier might impede a structural rearrangement between the two fully relaxed equilibrium ground state atomic configurations of the two charge states. Table 2 presents the defect levels computed with in LDA context (all results FDSM-extrapolated from 216-site cells to infinitely dilute bulk defects), and Table 3 presents the defect levels computed in the PBE context.

The first entry for Si_{In} (Si_{As}) in Table 2-3 is the explicit DFT calculated defect level using the site-shifted neutral reference, and the second entry is for the full prediction derived for the on-site dopant defect. Silicon is a shallow *n*-type dopant in InAs, sitting in the indium substitutional site, Si_{In}. Being a shallow donor, Si_{In} has a (1+/0) transition near the valence band edge. However, the DFT calculation buries this state into the conduction band and the $Si_{In}[0]$ (and its compensating partner $Si_{As}[0]$) is not a clean defect state, reflecting a DFT difficulty has treating shallow effective-mass-like states. To evaluate a formation energy for $Si_{In}[1+]$ ($Si_{In}[1-]$) from a total energy analysis, a clean neutral defect state is needed. This reference state is obtained by exchanging the silicon and a neighboring indium, to create a As_{In}-Si_{As} [In_{As}-Si_{In}] pair defect, designated as $Si^{x}_{In}(0)$ [$Si^{x}_{As}(0)$], which has a clean defect state with neutral charge. With this neutral defect and the charge transition energy, the formation energy of $Si_{In}[1+]$ (and $Si_{As}[1-]$) is obtained directly from the DFT calculations, without assumptions regarding the location of the (computationally inaccessible) shallow on-site transition. The formation energy of the charged substitutional is obtained by reference to the site-switched $Si^{x}_{In}(0)$ [$Si^{x}_{As}(0)$], and then, in turn, the *neutral* simple substitutional formation energy of Si_{In} [Si_{As}] is obtained from the charged defect by assuming that the level lies at the band edge, *assuming* a band gap of 0.42 eV (the experimental band gap for InAs).

Computed levels in the LDA and PBE contexts are very similar, all within 0.3 eV of one another, and mostly within 0.1 eV. The differences in Si-containing defect formation energies are also typically 0.2 eV, and is, first, evidence that LDA and PBE are giving consistent results and, second, consistent with—and evidence for—a physical uncertainty in defect levels of 0.1-0.2 eV.

The defect levels listed in these tables only quote those charge states that are thermodynamically accessible, plus additional states for comparison to the analogous defects in GaAs. For example, clean defect states for the $(AsSi)_{In}$ and Si_i can be found for [1-] and [2-] charge states and a *DX* (offset-Si) configuration for Si_{In}, is a clean defect state as a [1-] charge, but none of these is thermodynamically stable, they will spontaneously emit electrons to form the neutral defects. Alternatively stated, the electronic levels are above the CB edge, as a consequence of the energy gained in the structural rearrangements that occur. The Si interstitial levels are all above the InAs CBE, indicating that this defect is predicted to favor a [2+] charge state. These are included in the Table to facilitate comparisons to Si-doped GaAs, and thereby enable inferences about Si-doped ternary $In_xGa_{(1-x)}As$, which is the ultimate purpose of this study in Si-doped InAs.

Table 2. Defect levels for silicon reaction network defects, context = LDA.

LDA **Context**	**Neutral formation energy**	**Defect levels (eV), cf. VBE**				
		(3+/2+)	**(2+/1+)**	**(1+/0)**	**(0/1-)**	**(1-/2-)**
$Si^{x}_{In}(0)$ /$Si_{In}(+)$	**1.99**	-	-	2.24	-	-
Si_{In}	**(0.17)**	n/x	n/x	0.42^{CBE}	-	n/x
$Si_{As}(-)$/ **$Si^{x}_{As}(0)$**	**2.09**	n/x	n/x	n/x	-0.32	n/x
$Si_{As}^{(a)}$	**(1.35)**	n/x	n/x	n/x	0^{VBE}	n/x
Si_{i}	**3.31**	n/x	1.16	0.65	-	-
$(Si_2)_{In}$	**3.29**	0.64	0.07	0.89	0.37	n/x
$(AsSi)_{In}$	**2.34**	n/x	0.07	039	-	-
Si_{vv}	**2.77**	n/x	0.26	0.22	0.75	0.66

Table 3. Defect levels for silicon reaction network defects, context = PBE.

PBE **Context**	**Neutral formation energy**	**Defect levels (eV), cf. VBE**				
		(3+/2+)	**(2+/1+)**	**(1+/0)**	**(0/1-)**	**(1-/2-)**
$Si^{x}_{In}(0)$ /$Si_{In}(+)$	**2.14**	-	-	2.15	-	-
Si_{In}	**(0.37)**	n/x	n/x	0.42^{CBE}	-	n/x
$Si_{As}(-)$/ **$Si^{x}_{As}(0)$**	**2.35**	-	-	-	-0.39	-
Si_{As}	**(2.33)**	n/x	n/x	n/x	0^{VBE}	n/x
Si_{i}	**3.32**	n/x	1.25	0.64	-	-
$(Si_2)_{In}$	**3.17**	0.54	0.21	0.89	0.43	n/x
$(AsSi)_{In}$	**2.25**	n/x	0.17	0.46	-	-
Si_{vv}	**2.60**	n/x	0.47	0.24	0.85	0.72

2.3. Defect formation energies

The ground state defect formation energies, as a function of charge state are trivially obtained by simple arithmetic from the neutral formation energies and the computed defect charge transition energy levels presented in Table 2-3 in the previous section. As for all the results presented in this Report, the defect formation energies in the following Tables are presented in the arsenic-rich limit. For consistency with the intrinsic defect results [1], the formation energies of the charged defects are presented with a Fermi level set to be at the VBE. The Tables present the formation energies of the silicon reaction network defects, segregated by simulation context. Only thermodynamically accessible charge states are listed.

Table 4. Formation energies of silicon reaction network defects at VBE (in eV), context = LDA.

Charge state	Si_{In}	Si_{As}	Si_i	$(Si_2)_{In}$	$(AsSi)_{In}$	Si_{vv}
(2-)	-	-	-	-	-	4.18
(1-)	-	1.35	-	3.66	-	3.53
(0)	**(0.17)[a]**	**(1.35)[a]**	**3.31**	**3.29**	**2.34**	**2.77**
(1+)	-0.25	-	2.67	2.41	1.95	2.55
(2+)	-	-	1.51	2.33	1.88	2.29
(3+)	-	-	-	1.70	-	-

a) For T_d on-site $Si_{In}[0]$ and $Si_{As}[0]$, assuming a shallow level exactly at the respective band edges, and assuming a band gap of 0.42 eV (the experimental band gap for InAs).

Table 5. Formation energies of silicon reaction network defects at VBE (in eV), context = PBE.

Charge state	Si_{In}	Si_{As}	Si_i	$(Si_2)_{In}$	$(AsSi)_{In}$	Si_{vv}
(2-)	-	-	-	-	-	4.17
(1-)	-	1.40	-	3.60	-	3.45
(0)	**(0.14)[a]**	**(1.40)[a]**	**3.32**	**3.17**	**2.25**	**2.60**
(1+)	-0.28	-	2.68	2.28	1.78	2.36
(2+)	-	-	1.43	2.07	1.62	1.88
(3+)	-	-	-	1.53	-	-

a) For T_d on-site $Si_{In}[0]$ and $Si_{As}[0]$, assuming a shallow level exactly at the respective band edges, and assuming a band gap of 0.42 eV (the experimental band gap for InAs).

The formation energies for the CBE Fermi level consistent with the *n*-type character of Si doping in InAs is trivially obtained by simple arithmetic using a band gap energy. Tables 6-7 present the equivalent results to Tables 4-5, arithmetically re-referenced to have the Fermi level at the CBE, appropriate to *n*-type InAs given by Si doping, assuming a band gap of 0.42 eV for InAs.

Table 6. Formation energies of silicon reaction network defects at CBE (in eV), context = LDA.

Charge state	Si_{In}	Si_{As}	Si_i	$(Si_2)_{In}$	$(AsSi)_{In}$	Si_{vv}
(2-)	-	-	-	-	-	3.34
(1-)	-	0.93	-	3.24	-	3.11
(0)	**(0.17)[a]**	**(1.35)[a]**	**3.31**	**3.29**	**2.34**	**2.77**
(1+)	0.17	-	3.09	2.83	2.37	2.97
(2+)	-	-	2.34	3.17	2.72	3.13
(3+)	-	-	-	2.96	-	-

a) For T_d on-site $Si_{In}[0]$ and $Si_{As}[0]$, assuming a shallow level exactly at the respective band edges, and assuming a band gap of 0.42 eV (the experimental band gap for InAs).

Table 7. Formation energies of silicon reaction network defects at CBE (in eV), context = PBE.

Charge state	Si_{In}	Si_P	Si_i	$(Si_2)_{In}$	$(AsSi)_{In}$	Si_{vv}
(2-)	-	-	-	-	-	3.33
(1-)	-	0.98	-	3.18	-	3,03
(0)	**(0.14)[a]**	**(1.40)[a]**	**3.32**	**3.17**	**2.25**	**2.60**
(1+)	0.14	-	3.10	2.70	2.20	2.78
(2+)	-	-	2.27	2.91	2.46	2.72
(3+)	-	-	-	2.79	-	-

a) For T_d on-site $Si_{In}[0]$ and $Si_{As}[0]$, assuming a shallow level exactly at the respective band edges, and assuming a band gap of 0.42 eV (the experimental band gap for InAs).

2.4. Silicon interstitial and migration

In the evolution of the defect reaction network, as the mobile As and In interstitials react with the immobile fixed defects, the silicon interstitial is the only additional defect that shows a prospect to be also mobile, and therefore must be considered in extending the defect reaction network. The LDA and PBE structural landscapes for the silicon interstitial are similar to each other. The silicon interstitial strongly favors in-network sites when neutral, and favors non-bonding interstitial sites when positively charged, dissociating into an on-site atom (As or Si) and a nearby interstitial.

The Si interstitial favors in-network bonds in the neutral charge state that might dominate *n*-type InAs, although the current calculations suggest that the [2+] charge state will dominated for Fermi levels across the InAs band gap. A comprehensive assessment of diffusion for the neutral defect, computation of continuous pathways and explicit migration barriers, is likely impractical using a semilocal functional, because of extensive regions, particularly the non-network configurations, where the defect state crosses into the conduction band. However, thermal migration might be facile, with many configurations on the In site and the As site having energies within 1 eV of the ground state.

Unlike for the arsenic interstitial in GaAs [13], there is not an identified path that could mediate athermal diffusion [15] of the silicon interstitial via a Bourgoin-Corbett mechanism [16], in either the LDA or PBE context simulations. With the bistability with charge state—different metastable configurations having different relative stabilities with a change in charge state—however, one can anticipate that recombination-enhanced diffusion will contribute significantly to the diffusion of the Si interstitial. There is a possibility of athermal diffusion, an extreme limit of recombination-enhanced diffusion where there is no thermal barrier, as the Si interstitial changes from an in-network neutral defect to non-network ionized interstitial defect. Recombination-enhanced diffusion by this mechanism would likely be enabled in non-equilibrium radiation-damaged regions of InAs.

2.5. Defect network reaction energies

Using the defect formation energies tabulated above for the silicon-related defects, and the defect formation energies previously tabulated for intrinsic defects [1], it is straightforward to compute the defect reaction energies of possible reactions in the defect reaction network for Si-doped InAs. All reactions of the three potentially mobile species, the arsenic and indium self-interstitials and the silicon interstitials, with the common immobile defects, the vacancies and substitutional dopant, could be considered. The results for charge conserving reaction among intrinsic defects and also silicon-containing reactions are trivially obtained from the formation energies above, following the prescription used for collated reaction energies in GaAs presented in Ref. 14, and is not duplicated here.

3. CONCLUSIONS

The defect reaction network for *n*-type silicon-doped indium arsenide is developed, beginning with the interstitials mobilized in displacement damage, following the reactions with the immobile displacement damage defects and the dopant atoms, and culminating in immobile reaction products. The defect energies predicted with DFT are presented for each defect in the reaction network, and the computed properties needed to describe the each defect in the network—stable charge states, energy levels, formation energies—are tabulated. Both LDA and PBE results are presented. The results are only presented using "large-core" Z=3 In pseudopotentials and without spin polarization. The calculations could be straightforwardly repeated with the small-core Z=13 In pseudopotentials, and also to include spin.

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