Ab initio models of amorphous $Si_{1-x}Ge_x$: H

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We study the structural, dynamical, and electronic properties of amorphous $Si_{1-x}Ge_x$: H alloys using firstprinciples local basis molecular dynamics techniques. The network topology and defects in the amorphous network have been analyzed. Structural changes, particularly an increase in number of defects and strained bond angles, have been found as the Ge content increases from x=0.1 to 0.5. The electronic density of states exhibits a decreasing band gap and additional midgap and band-tail defect states as Ge concentration increases. We report the network structures which are responsible for midgap and band-tail states. The band tails show an exponential (Urbach) behavior. The mobility gap is coarsely estimated as a function of Ge concentration.

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I. INTRODUCTION

Hydrogenated amorphous Si-Ge alloys are important materials for uncooled microbolometer applications, especially "thermal" night vision and IR sensing.^{1,2} The materials are of basic interest as they exhibit a mild form of alloy disorder (here "mild" refers to the chemical similarity of the two species) juxtaposed with topological disorder. Since the band gap of these alloys can be tuned by changing composition, they are being used and explored for photovoltatic applications.^{3–5} The electrical, optical, and vibrational properties have been studied from experiment.^{6–9}

There are a number of experimental investigations on the bonding in amorphous Si_{1-x}Ge_x alloys (both with and without hydrogen). Using extended x-ray absorption Nishino *et al.*¹⁰ found the Ge-Ge and Ge-Si bond lengths to be independent of composition (2.46 and 2.41 Å, respectively). This is consistent with another x-ray absorption measurement by Incoccia *et al.*¹¹ a few years before. On the other hand, for the nonhydrogenated alloys researchers showed a linearly increasing bond length as a function of concentration^{12–15} opposing the idea of "composition independent" bond length. However, there is limited understanding of whether the difference is connected to the presence of hydrogen in the alloy or not.

There are many simulations of a-Si and a-Si:H.^{12,16–21} Most of these studies provide networks in reasonable agreement with experiment, using a variety of different approaches. Our aim here is to offer small but reliable models of a-SiGe:H alloys, studying the effect of Ge concentration on bond length and on the structure of the amorphous network. Wherever possible, we compare the models to experiment and make specific predictions of the structural origins of defect states appearing near the Fermi level. It seems likely that because of delicate energetics of alloy disorder, relaxation effects and (mild) charge transfer, a first-principles approach is needed.

The paper is organized as follows. In Sec. II, we discuss the approximations and parameters used in the *ab initio* code employed, and describe procedures for generating *a*-Si_{1-x}Ge_x:H alloy models. In Sec. III we describe the structural properties by studying partial pair correlations, atomic coordination, and bond angle distributions. The electronic properties of localized midgap and band-tail states are presented in Sec. IV. From the standpoint of band gap engineering, we describe the evolution of state density as a function of composition. The dynamical properties and vibrational density of states are given in Sec. V. Finally, we present conclusions.

II. METHODOLOGY

A. Total energy and forces

The density functional calculations in the present work were performed within the generalized gradient approximation²² (GGA) using the first-principles code SIESTA.²³ Calculations in this paper employed a single ζ basis with polarization orbitals (SZP) for Si and Ge and a double ζ polarized basis (DZP) for hydrogen.²⁴ The structures were relaxed using conjugate gradient (CG) coordinate optimization until the forces on each atom were less than 0.02 eV/Å. We solved the self-consistent Kohn-Sham equations by direct diagonalization of the Hamiltonian and a conventional mixing scheme. The $\Gamma(\vec{k}=0)$ point was used to sample the Brillouin zone in all calculations.

B. Model formation

Realistic models of a-Si have been obtained from the Wooten-Weaire-Winer (WWW) algorithm.²⁵ To model hydrogenated structures, we developed a 223-atom a-Si:H model by removing two Si atoms and adding nine H atoms (of the fourfolded 216-atom a-Si) to terminate all the dangling bonds except one (to enable the observation of one dangling bond defect). Each of the H atoms were placed about 1.5 Å from the corresponding threefold Si atom. This model is relaxed using the conjugate gradient method. After relaxation, we replaced some of the Si atoms by Ge atoms at random, and then relaxed the cell to generate $a-Si_{1-r}Ge_r$:H alloys, with the Ge fraction *x* being 0.1, 0.2, 0.3, 0.4, and 0.5. We note that our models have the advantage that they are a minimum for an accurate energy functional. On the other hand, because of the *a priori* assumption of a tetrahedral a-Si network, and no possibility for modeling diffusive pro-



FIG. 1. (Color online) Si-Si, Si-Ge, and Ge-Ge bond lengths as a function of Ge concentration. The straight lines with triangle up and triangle down symbols are experimental values of Si-Ge and Ge-Ge bond lengths, respectively, taken from Nishino *et al.* (Ref. 10).

cesses because of the rapid descent into a minimum, it is likely that our models will tend to underestimate disorder effects associated with alloying. Like other calculations of this sort the justification is partly *a posteriori*: namely agreement with a variety of experiments.

III. STRUCTURE

A. Bond length and pair correlation functions

For a given Ge atomic composition, *x*, we obtained the average bond lengths between Si-Si, Si-Ge, and Ge-Ge. In Fig. 1 we show these bond lengths as a function of Ge composition. The experimental data which are obtained for Ge composition $x \ge 0.3$ from Nishino *et al.* are shown in Fig. 1. By taking an average value of each type of bond for all the compositions, we obtained a mean bond length value of 2.42 Å for Si-Ge and 2.46 Å for Ge-Ge bonds compared with the experimental values of 2.46 and 2.41 Å.^{10,14} Our result gives a mean bond length of 2.37 Å for the Si-Si bond which is again in the experimental range of 2.35–2.37 Å.²⁶

The topology of models may be analyzed by partial pair correlation functions $g_{\alpha\beta}(r)$ of atomic species α and β . The partial pair correlation $g_{\alpha\beta}(r)$ can be written as

$$g_{\alpha\beta}(r) = \frac{1}{4\pi r^2 \rho N c_{\alpha} c_{\beta}} \sum_{i \neq j} \delta(r - r_{ij}), \qquad (1)$$

where N is the total number of particles in the system; $\rho = \frac{N}{V}$ is the number density, $c_{\alpha} = \frac{N_{\alpha}}{N}$, and $c_{\beta} = \frac{N_{\beta}}{N}$. We have used a Gaussian approximation for the delta function with broadening $\sigma = 0.1$ Å.

We have analyzed the five alloy compositions, and a first nearest neighbor peak with subsequent deep minimum is always evident. These features imply strong short-range ordering in the models. In Fig. 2 we plot the partial pair correla-



FIG. 2. (Color online) Partial pair distribution function $g_{\alpha\beta}$ of a-Si_{1-x}Ge_x:H alloys for two compositions (x=0.1 and 0.5): (a) Si-Si, (b) Ge-Ge, and (c) Si-Ge.

tion for Si-Si, Ge-Ge, and Si-Ge in the a-Si_{1-x}Ge_x:H alloy for x=0.1 and 0.5. For Ge-Ge we obtained a first peak at $r_o \sim 2.46$ Å which is the same for the two compositions considered. Similarly, the partial correlation for Si-Ge has a first peak at 2.42 Å and Si-Ge has first peak at 2.37 Å. We observed considerable similarity in first nearest neighbor peaks for the various Ge concentrations. These results support and reproduce values observed in experiment.^{10,14,26} Our models retain an essentially tetrahedral structure for all Ge concentrations, albeit with defects and strain increasing with x.

B. Geometry of bonding

The tetrahedral *a*-Si (WWW) model ancestral to the alloy models we present here is fully coordinated (fourfold coordination for all the Si atoms). Thus random substitution of Ge without relaxation preserves the fourfold tetrahedral structure. The essential difference between the model with random substitution (without relaxing) and the fully relaxed case (the models we present in this paper) is that we see a decrease in the number of fourfold atoms (through creation of both threefold and fivefold atoms) as the Ge content increases. There is also an increase in weak (long) bonds. These changes influence all physical properties of the alloy systems. Like any *ab initio* simulation, the detailed numerics of our calculations must be taken with a grain of salt: the systems, while large by the standards of first-principles studies, do not provide statistical error bars on coordination and defects. It is reasonable, however, to expect general trends to be reproduced as a function of x.

TABLE I. The value of r_o in the first peak of the g(r) and the first neighbor coordination number $n_{\alpha\beta}$ in a-Si_{1-x}Ge_x: H alloys for five different Ge atomic compositions x=0.1-0.5. The integration ranges are from 0.0 to 2.8 Å for Si-Si, Ge-Ge, Si-Ge, and Ge-Si and 0.0–1.8 Å for Si-H, Ge-H, H-Si, and H-Ge.

		$n_{\alpha\beta}$ for first shell						
Bond type	$\stackrel{r_o}{({ m \AA})}$	<i>x</i> =0.1	<i>x</i> =0.2	<i>x</i> =0.3	<i>x</i> =0.4	<i>x</i> =0.5		
Si-Si	2.37	3.47	3.07	2.70	2.37	2.06		
Si-Ge	2.42	0.50	0.86	1.22	1.54	1.97		
Si-H	1.53	0.04	0.05	0.05	0.05	0.06		
	n _{Si}	4.01	3.98	3.97	3.96	4.09		
Ge-Ge	2.46	0.16	0.71	1.11	1.58	1.92		
Ge-Si	2.42	3.80	3.22	2.80	2.34	2.04		
Ge-H	1.60	0.04	0.02	0.03	0.02	0.03		
	n _{Ge}	4.00	3.95	3.94	3.94	3.99		
H-Si	1.53	0.89	0.89	0.78	0.78	0.67		
H-Ge	1.60	0.11	0.11	0.22	0.22	0.33		
	$n_{\rm H}$	1.00	1.00	1.00	1.00	1.00		

We obtained partial n_{Ge} , n_{Si} , n_{H} , and average coordination numbers, n, based on the nearest neighbor distance determined in the preceding section; first neighbor coordination numbers n_{SiSi} , n_{SiGe} , n_{SiH} , n_{GeGe} , n_{GeSi} , and n_{GeH} are obtained by integrating the pair correlation function $4\pi r^2 \rho g_{\alpha\beta}(r)$. The results are shown in Table I. The total coordination numbers for Ge, Si, and H are $n_{\text{Ge}} = n_{\text{GeGe}} + n_{\text{GeSi}} + n_{\text{GeH}}$, $n_{\text{Si}} = n_{\text{SiSi}} + n_{\text{SiGe}} + n_{\text{SiH}}$, and $n_{\text{H}} = n_{\text{HSi}} + n_{\text{HGe}}$, respectively. The observation of higher coordination number for composition x=0.5 is due to a net increase in overcoordinated (fivefold) bonds versus under-coordinated (threefold) bonds. It is not obvious that total coordination of 4.09 at x=0.5 is statistically significant; this will be checked in future work with extended annealing studies. The salience of these changes to the electronic structure of the alloy is discussed in Sec. IV.

To investigate the effect of Ge composition on the structures, we analyzed and obtained all types of bonding and structures in the network for each Ge composition considered. For x=0.1, about 96.81% of Si and 95.83% of Ge are fourfold, only 1.06% of Si and 4.17% of Ge are threefold coordinated, 2.13% of Si are fivefold. No fivefold coordination is obtained for Ge. Where fourfold Si is concerned, Si₄ (a Si atom bonded with four Si atoms) is a dominant structure which is followed by Si₃Ge (a Si atom bonded with three Si and one Ge atoms). We observed a similar pattern in the Ge fourfold coordination that Ge bonded to Si₄ structure is highly dominant which is followed by Ge bonded with Si₃Ge. The detailed results are shown in Table II.

In the case of x=0.5, we observed ~10.47% fivefold bonds for Si. About 87.21% of Si and 99.04% of Ge are fourfold, only 2.33% of Si and 0.96% of Ge are threefold coordinated. The dominant structure in this case is a Si atom bonded with Si₂Ge₂, followed by Si₃Ge. A similar pattern is observed in the Ge fourfold atoms. The results are shown in Table III. Comparing the bonding statistics of the relaxed network with the initial configuration (in which we randomly substituted Ge for Si), we see a significant decrease in the number of fourfold atoms. Also, we observe an increase in the number of weak bonds (~9.5%) for the case of x=0.5. The increase in weak bonds in this case is relative to the number of such bonds in the case of x=0.1. Here, weak bond refers to a Si-Si or Si-Ge bond with bond length between 2.5 and 2.7 Å.

TABLE II. Average percentage $m_{\alpha}(l)$ (bold characters) of atoms of species Si and Ge, *l*-fold coordinated at a distance of 2.68 Å for both Si and Ge, and 1.55 Å for H in a-Si_{1-x}Ge_x:H alloy for Ge atomic composition x=0.1. We also give the identity and the number of Ge and Si neighbors for each value of $m_{\alpha}(l)$.

Si				<i>l</i> =3	1.06
				Si ₃	0.53
				Si ₂ Ge	0.53
l=4	96.81	<i>l</i> =5	2.13		
Si ₄	52.67	Si ₅	1.06		
Si ₃ Ge	32.98	Si ₄ Ge	1.06		
Si ₂ Ge ₂	6.91				
Si ₃ H	3.72				
Si ₂ GeH	0.53				
Ge		<i>l</i> =3	4.17	l=4	95.83
		Si ₃	4.17	Si_4	79.17
				Si ₃ Ge	12.50
				Si ₂ GeH	4.17

TABLE III. Average percentage $m_{\alpha}(l)$ (bold characters) of atoms of species Si and Ge, *l*-fold coordinated at a distance of 2.68 Å for both Si and Ge, and 1.55 Å for H in a-Si_{1-x}Ge_x:H alloy for Ge atomic composition x=0.5. We also give the identity and the number of Ge and Si neighbors for each value of $m_{\alpha}(l)$.

Si				<i>l</i> =3	2.32
				Si ₂ Ge	1.16
				Si ₃	1.16
<i>l</i> =4	87.21	<i>l</i> =5	10.47		
Si ₂ Ge ₂	51.16	Si ₄ Ge ₁	3.49		
Si ₃ Ge ₁	19.77	Si ₃ Ge ₂	5.81		
Ge ₄	8.14	$\rm Si_4H$	1.16		
Si ₄	5.81				
Si ₃ H	1.16				
Si ₂ GeH	1.16				
Ge				<i>l</i> =3	0.96
				Si ₂ Ge	0.96
<i>l</i> =4	99.04				
Si ₂ Ge ₂	40.38				
Si ₃ Ge	26.92				
SiGe ₃	21.15				
Si ₄	3.85				
Ge ₄	3.85				
Ge ₂ SiH	1.92				
Ge ₃ H	0.96				

Angular distribution

We calculated the partial angular distributions for *a*-Si_{1-x}Ge_x:H with x=0.1, 0.3, and 0.5 Ge compositions and plotted them in Figs. 3(a)-3(f). Though we report only three



Ge compositions, the trends are similar for the other two Ge compositions x=0.2 and 0.4. The partial pair correlation functions for α -Si- γ are plotted in the upper panel and the partial pair correlation functions for α -Ge- γ are plotted in the lower panel. In each of the cases considered, we found total angular distribution peaks centered near the tetrahedral angle with θ in the range 103°–110°. The broader angular distributions for Ge-Si-Si and Ge-Ge-Si as the Ge concentration increases represent departures from the highly tetrahedral network we began with. We also report information on partial angular distributions for H. The mean of the distribution of H-Si-Si and H-Ge-Ge is close to the tetrahedral angle 109.47° while the other two partials, H-Ge-Si and H-Si-Ge, deviate from a tetrahedral angle and range from 100.0° to 116.0°. In general, our results show broader angular distributions (far from a tetrahedral angle of 109.47°) in the case of H-Ge-Si and H-Si-Ge, where atoms of three different species form an angle. This is presumably connected to the asymmetries in bonding associated with the distinct species. This feature has also been observed in the case of structures, Ge-Si-Si and Ge-Ge-Si. As shown in Fig. 3 we observe a broader angular distribution for the two structures as the Ge composition increases. The probability density for $\cos(\theta)$ is normal (Gaussian), which is characteristic of all WWW models (and may indeed be more general). As reported elsewhere, normally distributed cosines of bond angles lead easily to exponential (Urbach) band tails in the electron density of states near the valence and conduction edges.²⁷ We return to this point in the discussion of the electronic density of states.

IV. ELECTRONIC STRUCTURE

A. Density of states

Electronic structure has been described by the electronic density of states (EDOS), which was obtained by summing

FIG. 3. (Color online) The partial bond-angle distribution function as a function of bond angle θ in *a*-Si_{1-x}Ge_x:H for *x*=0.1 (left panel), for *x*=0.3 (middle panel), and for *x*=0.5 (right panel). (a)–(c) are partial angular distribution for three possible angles centering Si and (d)–(f) are partial angles taking Ge as a center.



FIG. 4. (Color online) The electron density of states for $a-\text{Si}_{1-x}\text{Ge}_x$: H for x=0.4. The exponential fit in the inset for the valence band tail is $2.5 \times e^{-E/E_o}$ with $E_o=192$ meV for x=0.4. The Fermi level is shifted to E=0, units: eV^{-1} .

suitably broadened Gaussians centered at each Kohn-Sham eigenvalue.²⁸ The results showed a band gap (~1.6 eV for x=0.1) that becomes narrower as the Ge composition increases (~0.8 eV for x=0.5). As usual, the reader should remember that the local density approximation (LDA) gaps reported in this paper are significantly smaller than experiment. It is expected that trends with composition should be reproduced, however.

In this section, we present the results of one of the alloys (for $a-\text{Si}_{1-x}\text{Ge}_x$: H with x=0.4) among the five different Ge atomic compositions. The electron density of states (EDOS) shown in Fig. 4 shows a narrow gap. The band tails of the spectrum which we take in the region (-0.7-0.0 eV) fits exponentially with $\sim e^{-E/E_o}$ with $E_o=192 \text{ meV}$ as shown in the inset of Fig. 4. We analyze these defect states in the spectrum in detail in the next sections.



FIG. 5. (Color online) Inverse participation ratio (IPR) in the a-Si_{1-x}Ge_x:H alloy for x=0.1 vs energy. The dashed line is the Fermi level.



FIG. 6. (Color online) The contribution of atoms to the IPR (10% and above) of a given state in a-Si_{1-x}Ge_x:H alloy for x=0.1. The labels from a to f correspond to different mid gap and band-tail states of Fig. 5.

B. Localization: Inverse participation ratio

In order to understand the electron localization we used the inverse participation ratio (IPR),

$$IPR = \sum_{i=1}^{N} [q_i(E)]^2,$$
 (2)

where $q_i(E)$ is the Mulliken charge residing at an atomic site *i* for an eigenstate with eigenvalue *E* that satisfies $\sum_{i}^{N}[q_i(E)]=1$ and *N* is the total number of atoms in the cell. For an ideally localized state, only one atomic site contributes all the charge and so IPR=1. For a uniformly extended state, the Mulliken charge contribution per site is uniform and equals 1/N and so IPR=1/N. Thus large IPR corresponds to localized states, small IPR to extended states.

To investigate how the electronic properties evolve with composition in the gap, we have calculated the IPR of a- $Si_{1-x}Ge_x$: H alloy for two different Ge compositions, x=0.1and 0.4. We have determined the individual atomic contributions to the total IPR for localized eigenstate, to associate that state with particular structural irregularities. This provides a "spectral signature" for the various defect structures that emerge in our models. Since we are interested in states near the Fermi level, we limit our presentation here only to eigenvectors conjugate to eigenvalues which are midgap or near the band tails of the spectrum. We plotted the inverse participation ratio and the contributions of each of the atoms to the IPR for x=0.1 in Figs. 5 and 6, respectively. For the IPR, we only chose those atoms which contribute 10% or more for a particular state labeled a-f. Those structures in the alloy which correspond to the selected midgap and band-tail states labeled a-f are shown in Fig. 7. As we can see from Fig. 5, there is one midgap state and about five band-tail states. We estimated the mobility band gap in this case to be ~1.6 eV.



FIG. 7. (Color online) Representation of selected electronic eigenstates labeled in Fig. 5 from a to f in the a-Si_{1-x}Ge_x:H alloy for x=0.1. The color code is cyan (light gray) for Si and violet (dark gray) for Ge. Numbers indicate selected site contributions to the eigenstate.

The structures which are responsible for the midgap state labeled c, arise from a threefold Si, a fivefold Ge, and defects. Note that the state is not entirely centered upon one obvious defect (there is resonant mixing) as predicted by the resonant cluster proliferation model.²⁹ We have also determined the structures corresponding to the band-tail states (a, d, and e). The large IPR derives primarily from a structure involving three fourfold Si but nontetrahedral sites ($\delta\theta \approx 15^{\circ}$). The other two midgap states come from a fivefold Si atom together with a strain defect (b), and a threefold Si bonded with a fivefold Si and a geometrical defect (f).

In the case of x=0.4, the inverse participation ratio as a function of eigenvalue is plotted in Fig. 8, while the contributions of each of the atoms to the IPR (only those atoms which contribute 5% and more) for a particular state labeled a–f and the different structures associated with these states are plotted in Figs. 9 and 10, respectively. As we can see

from the IPR plots in the two cases, x=0.1 and 0.4, as the Ge content increases, we observed an increasing number of band-tail states close to the conduction band edge and hence a narrow band-gap spectrum.

By comparing the models for various *x*, we observe that strain defects become important in accounting for the band tail states for increasing Ge content. As shown in Fig. 10, large contributions to the state labeled (a) and (b) come from geometrical defects, a fivefold Si, and a threefold Ge structure. States labeled (d) and (f) in this case are dominated by a geometrical defect which has three fourfold Si atoms connected to each other with a strained bond with angular distribution off from a tetrahedral angle by $\pm 20^{\circ}$. The dominant contributions to the midgap state arise from a fivefold Si atom bonded with two strain defects.

To emphasize the effect of Ge concentration in the mobility band gap, we have estimated the mobility gap as a func-



FIG. 8. (Color online) Inverse participation ratio (IPR) vs energy in a-Si_{1-x}Ge_x: H alloy for x=0.4. The dashed line is the Fermi level.

tion of the Ge concentration x in Fig. 11(f). The mobility gaps are extracted from Figs. 11(a)-11(e) which show the inverse participation ratio as a function of eigenvalues for different x. We observed a decrease in the mobility gap as the Ge concentration increased from x=0.1 to 0.5. The mobility gap is roughly estimated by examination of the plots of IPR versus energy. In each case, there is a fairly well-defined energy near the valence and conduction tails at which the IPR becomes roughly constant reflecting the onset of extended states. We include "error bars" to convey a rough estimate of uncertainty in our estimated gaps.

V. DYNAMICAL PROPERTIES

The lattice dynamics of a-Si_{1-x}Ge_x: H alloys are analyzed with the vibrational density of states (VDOS) and inverse



FIG. 9. (Color online) The contribution of atoms to the IPR (5% and above) of a given state in a-Si_{1-x}Ge_x:H alloy for x=0.4. The labels from a to f correspond to different midgap and band-tail states of Fig. 8.



FIG. 10. (Color online) Representation of selected electronic eigenstates labeled in Fig. 8 from a to f in the a-Si_{1-x}Ge_x:H alloy for x=0.4. The color code is cyan (light gray) for Si and violet (dark gray) for Ge. Numbers indicate selected site contributions to the eigenstate.

participation ratio. The vibrational eigenvalues and eigenvectors are obtained by diagonalizing the dynamical matrix. The dynamical matrix is determined by displacing each atom with 0.03 Å in three orthogonal directions and then performing first-principles force calculations for all the atoms for such displacement. Each calculation yields a column of force constant matrix.

In Fig. 12, the phonon density of states for $a-Si_{1-x}Ge_x$: H for x=0.4 is plotted. From our simulation, the



FIG. 11. (Color online) Inverse participation ratio (IPR) vs energy for different *x*: (a)–(e) and the estimated LDA mobility gap plotted vs the Ge concentration *x*: (f), in the a-Si_{1-x}Ge_x:H alloy. The red arrows indicate approximate mobility edges in the x=0.1 model.



FIG. 12. (Color online) Vibrational density of states (dashed) and the inverse participation ratio (blue) for the a-Si_{1-x}Ge_x:H model for x=0.4, units are meV⁻¹.

three optical mode peaks appear at 31.98 meV (Ge-Ge), 49.01 meV (Ge-Si), and 57.63 meV (Si-Si). The experimental results reported by Mackenzie *et al.*⁹ are 33.48, 45.87, and 58.27 meV for the three optical modes, respectively.

The higher frequency modes in the range (213-236 meV) are associated with hydrogen atoms with H-Si and H-Ge bonds which is in agreement with the experimental result (233.96 and 249.09 meV) reported by Wells *et al.*³⁰ The principal hydrogen related features of the spectrum which exhibit higher IPR (highly localized states) are stretch modes of Si-H at 252.81, 249.58, 245.49, and 232.22 meV, and of Ge-H at 236.07 and 204.08 meV, and a wagging vibration

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mode of Si-H and Ge-H dominates in the region of 74.39–111.59 meV.

The important experiments of Aljishi and co-workers⁶ provide basic information about the temperature dependence of the band-tail states of these materials. In subsequent work, we will explore the band-tail broadening from thermal motion³¹ and analyze the validity of the model for Urbach tailing in Ref. 27. The temperature-dependence of the band tailing is likely to be of significant interest for applications.

VI. CONCLUSION

We have presented an *ab initio* study of a-Si_{1-x}Ge_x:H alloys for five different Ge atomic compositions. Where the structural properties of a-Si_{1-x}Ge_x:H alloys are concerned, we show (a) a composition independent bond length, a modest, possibly statistically insignificant change in the total coordination, and total bond angle distribution, and (b) the emergence of geometrically strained structures and coordination defects as the Ge content increases. The electronic density of states shows an associated increase in band-tail state and gap states. This illustrates the process of "band gap engineering" with a clear illustration of how the gap closes (and with which states contributing) in the a-Si_{1-x}Ge_x:H alloy.

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