Corrigendum

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Parthapratim Biswas and Rajendra Timilsina
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Figure 1(a) in the paper was incorrectly printed, and should be replaced by the figure below.

Figure 1. (a) The presence of a monovacancy at low concentration (7\% H) in a region with four monohydrides (SiH).
Vacancies, microstructure and the moments of nuclear magnetic resonance: the case of hydrogenated amorphous silicon

Parthapratim Biswas and Rajendra Timilsina

Department of Physics and Astronomy, The University of Southern Mississippi, Hattiesburg, MS 39406, USA

E-mail: Partha.Biswas@usm.edu

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Abstract
Recent experiments on hydrogenated amorphous silicon using infrared absorption spectroscopy have indicated the presence of mono- and divacancies in samples for concentrations of up to 14% hydrogen. Motivated by this observation, we study the microstructure of hydrogen in two model networks of hydrogen-rich amorphous silicon with particular emphasis on the nature of the distribution (of hydrogen), the presence of defects and the characteristic features of the nuclear magnetic resonance spectra at low and high concentrations of hydrogen. Our study reveals the presence of vacancies, which are the built-in features of the model networks. The study also confirms the presence of various hydride configurations in the networks, from silicon monohydrides and dihydrides to open chain-like structures, that have been observed in the infrared and nuclear magnetic resonance experiments. The broad and the narrow line widths of the nuclear magnetic resonance spectra are calculated from a knowledge of the distribution of spins (hydrogen) in the networks.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

The distribution of hydrogen plays a very important role in determining the structural and electronic properties of amorphous silicon [1–6]. Hydrogen improves the electric properties of amorphous silicon by reducing the defect density via passivation [7, 8]. Fundamental to the understanding of the Staebler–Wronski (SW) [9–11] effect is the distribution and the dynamics of hydrogen atoms in amorphous silicon. An understanding of the local environment and the dynamics of various hydride configurations is therefore necessary to address the changes in the network structure and the properties brought about by the addition of hydrogen. Experimentally, the subject has been studied extensively via nuclear magnetic resonance (NMR) [12–17] and infrared (IR) spectroscopy [12, 13, 18, 19]. A proton magnetic resonance study [13] indicates that the distribution is inhomogeneous, and hydrogen can reside in the network as small clusters and in a dilute environment. Multiple-quantum NMR experiments [14] confirm that for device-quality samples a characteristic feature of the microstructure is the presence of small clusters (of four–seven H atoms), and at high concentration these clusters can merge to form large clusters. IR spectroscopy, on the other hand, can detect the presence of various hydrogen-bonding configurations by measuring the vibrational frequencies of hydrogen in the network. The IR studies by Ouwens and Schropp [19] indicate that for device-quality samples, 3–4% of total hydrogen atoms reside in the network as isolated or distributed monohydrides (SiH). The experiments by Manfredotti et al [18] and Lucovsky et al [20] provide evidence of the presence of various hydride configurations such as SiH, SiH2 and SiH3 in device-quality samples at low concentration. Likewise, at high concentration it has been observed that the networks can have open chains of...
behind the approach is to construct a series of guesses of as well) of the material under study. The principal idea available information (mostly experimental but other sources combine the power of a first-principles force field with the method is hybrid in the sense that it has the ability to constrained molecular relaxation (ECMR) method [32]. We amorphous silicon using a variant of the experimentally the construction of two model configurations of hydrogenated paper is organized as follows. In section 2, we briefly describe the experiments of Wu et al [26, 27] have recently addressed hydrogen–hydrogen pair separation in various dihydride configurations. The theoretical studies by Kim et al [29, 30] focused on some properties of vacancy configurations, such as the changes in the volume of a vacancy upon relaxation of the network. Zhang et al [31] studied the creation of higher order vacancies and their stability by relaxing the network from first-principles calculations. The latter study showed that any higher order vacancy had the tendency to evolve into a lower order vacancy including a monovacancy and a stable divacancy. However, an unsatisfactory feature of most of these theoretical studies was that the vacancies or defect conformations were created by hand and were then relaxed locally or globally in order to obtain a ‘stable’ vacancy configuration. While such an approach might be useful in studying the network structure and the local dynamics of the defect conformations, a short local or global relaxation may not be sufficient to eliminate the initial bias associated with the defect creation in an overconstrained network.

The purpose of the present work is to study the microstructure of hydrogen-rich amorphous silicon with particular emphasis on the presence of mono- and divacancies that have been observed recently via IR absorption spectroscopy [21]. The calculation of the line width of the resonance spectrum is also addressed using the second and the fourth moment of the resonance spectrum. We demonstrate that the inclusion of the fourth moment is particularly important in describing a highly inhomogeneous distribution of hydrogen observed recently in the experiments of Wu et al [15]. To this end, the rest of the paper is organized as follows. In section 2, we briefly describe the construction of two model configurations of hydrogenated amorphous silicon using a variant of the experimentally constrained molecular relaxation (ECMR) method [32]. We then address the presence of vacancies in the networks and compare the results to the recent experiments in section 3. This is followed by a brief discussion of the local environment of hydrogen atoms at low and high concentration in section 4. Section 5 addresses the calculation of the line width of the NMR spectrum using the Van Vleck moments going beyond the second moment (Gaussian) approximation [33].

2. Model generation: the ECMR approach

The ECMR is a hybrid approach developed by Biswas and Drabold [32], and has been applied to model a number of complex glassy systems in recent years [32, 34, 35]. The method is hybrid in the sense that it has the ability to combine the power of a first-principles force field with the available information (mostly experimental but other sources as well) of the material under study. The principal idea behind the approach is to construct a series of guesses of the solution (i.e. configuration) that are consistent with the available experimental data and an appropriate force field. These approximate solutions are then refined in an augmented solution space, which is a direct product of the configuration space of a potential (either empirical or first-principles) and that of the solution space feasible to the input experimental data. The imposition of suitably constructed prior information reduces the volume of the search space by hierarchically constructing a more probable solution space, and the system is driven to find the best solution in this subspace.

For the purpose of modeling hydrogenated amorphous silicon, a variant of the ECMR method has been used. The details of the method and its implementation in the context of modeling a-Si:H was described in [34]. Here we briefly mention the characteristic features of the method. The ECMR has been implemented as a two-step process that involves reverse Monte Carlo [36] followed by first-principle relaxations. The first step consists of packing Si atoms randomly into a cubic supercell subject to the constraint that no two Si atoms are closer than 2.0 Å to each other. Periodic boundary conditions are employed, and the density of the supercell is adjusted to match with the experimental density of amorphous silicon. A quadratic penalty function is used to incorporate experimental pair correlation data along with a set of constraints that describe the chemical and geometrical properties of the networks. The minimization of the penalty function provides a set of amorphous silicon co-ordinates, which is used to hydrogenate the network in the next step. Hydrogenation proceeds following a scheme similar to but not identical to that used by Holender, Morgan and Jones [37]. The hydrogenated networks are relaxed several times during the second step to ensure that the total force on the atoms is less 0.007 eV Å⁻¹. The relaxation is performed using SIESTA, which is a first-principles density functional code based on a local basis. Silicon atoms are treated using a minimal single-ζ (SZ) basis, whereas a double-ζ with polarization (DZP) orbitals is employed to represent the correct bonding behavior and hydrogen interaction accurately [34]. The typical size of the models is chosen to be of the order of 500 atoms, which is found to be sufficiently large to show no finite size effects but small enough to relax by the first-principles density functional code SIESTA.

The models used in the present study were previously validated thoroughly by comparing their structural, electronic and vibrational properties to the experimental data [34]. In this work, we focus on the predictive study of hydrogen distribution with particular emphasis on the presence of vacancies and the calculation of the line width of the NMR spectrum of these validated models. In particular, we consider two model configurations at low and high concentration that consist of 540 and 611 atoms, respectively. The 540-atom model has 7% H with 2.9% defect concentration consisting of dangling and floating bonds. The average co-ordination number of the network is 3.98. The model with high concentration has 22% H and a single defect of a two-fold Si atom. Both the models have a clean electronic band gap and the correct vibrational density of states. In the next few sections we demonstrate further that these model configurations are not only consistent
with structural, electronic and vibrational properties, but also with the NMR data as far as the shape and the width of the resonance spectra are concerned.

3. Vacancies in hydrogenated amorphous silicon

Unlike crystalline materials where vacancies can be defined uniquely and identified readily, the presence of disorder makes vacancy definition difficult in amorphous materials. Nonetheless, for continuous random networks, one can consider the missing of one or two neighboring atoms in the topologically connected environment as a mono- or a divacancy, respectively. Recent experiments on hydrogenated amorphous silicon samples prepared via an expanding thermal plasma technique by Smets et al.[21] have indicated that the microstructure in hydrogen-rich amorphous silicon can be characterized by the presence of vacancies and voids that largely depend on the amount of hydrogen present in the samples. In particular, these authors have observed that the microstructure is dominated by mono- and divacancies at low concentration of up to 14% H, whereas microvoids or voids appear at high concentration. Motivated by this experimental result, our interest lies in characterizing the microstructure (of our models) by searching for mono- and divacancy conformations that might be present in the models. It should be noted that in most of the theoretical studies [29–31], vacancies were explicitly introduced by hand in pure amorphous silicon networks, and the stability of the (vacancy) conformations was studied by relaxing the networks using an appropriate ab initio or tight-binding energy functional. A real-space analysis of the ECMR networks indeed confirms that both mono- and divacancies exist in the models. This observation is remarkable as vacancies are built-in or inherent in the networks, and are not introduced or generated locally as in most of the earlier theoretical works. These vacancies are a characteristic feature of the models, which is a direct consequence of our unique model building approach via ECMR [32]. In figure 1(a), we have shown the region surrounding the monovacancy that consists of four neighboring hydrogen atoms observed in the model with 7% H atoms. For clarity of presentation and to demonstrate the origin of the monovacancy clearly, we have explicitly shown the missing silicon atom in the reconstructed network in figure 1(b).

The presence of divacancies has been also found in our models. The observed divacancies can be divided into two types: stable and split [31]. For the latter, the two missing silicon atoms are not nearest neighbor but they are in close proximity of each other, typically within a distance of up to second nearest neighbors. In figure 3(a), we have shown the region consisting of a cluster of monohydrides at low concentration (7% H). The positions of the two (hypothetically) missing silicon atoms are shown in figure 3(b).

4. Hydrogen microstructure at low and high concentration

A review of the experimental literature suggests that hydrogen can reside in various bonding environments, which typically consist of SiH, SiH₂, SiH₃ [19, 18], and the chain structures of mono- and dihydrides that are connected via Si atoms [20]. The model with 7% H can be considered as a close approximation

1 The positions of the missing silicon atoms are obtained by removing the hydrogen atoms and introducing silicon atoms in the region. The resulting network is then relaxed via the first-principles density functional code SIESTA [40] to obtain the final configuration.
Figure 2. (a) A monovacancy at high concentration (22% H) in a region with several monohydrides (SiH). (b) The reconstructed network shows the missing silicon atom (in white). Silicon and the hydrogen atoms are shown in green (large) and yellow (small), respectively.

Figure 3. (a) A split divacancy with six monohydrides (SiH) at low concentration (7% H). (b) The origin of the divacancy is illustrated by showing the hypothetically missing two silicon atoms in the network (in white). Silicon and the hydrogen atoms are shown in green (large) and yellow (small), respectively.

Figure 4. (a) A stable divacancy at high concentration (22% H). (b) The reconstruction of the two missing silicon atoms (white) as described in the text. Silicon and the hydrogen atoms are shown in green (large) and yellow (small), respectively.

to a device-quality sample. For this value of concentration, most of the hydrogen atoms are found to be bonded to silicon atoms as monohydrides (SiH) and dihydrides (SiH$_2$). A total of 75% of all hydrogen atoms in the network is found to reside in the form of monohydrides, whereas the remaining 25% are realized in dihydride configurations. Furthermore, an examination of the model reveals that approximately 5% of the total hydrogen atoms in the network reside as isolated monohydrides. This result is in agreement with the experiment of Ouwens and Schropp [19], who have observed approximately 4% of total hydrogen atoms in the isolated phase. An example of such an isolated monohydride (SiH) realized in our model is shown in figure 5(a). The silicon complex in figure 5(a) consists of about 45 Si atoms within a radius of 6.0 Å surrounding the isolated hydrogen atom. Apart from such an isolated monohydride configuration, many of the monohydrides and the dihydrides are realized in the network that are close to each other, forming a dilute distribution of hydrogen. The remaining hydrogen atoms form clusters that typically consist of four–seven H atoms, which is consistent
Figure 5. (a) An isolated monohydride at low concentration (7% H) in a silicon complex of radius 6.0 Å. (b) A sparse distribution of hydrogen at low concentration showing six H atoms in a complex of radius of 6.0 Å. Silicon and hydrogen atoms are shown in green (large) and yellow (small), respectively.

Figure 6. (a) A pair of lone monohydrides realized in a dilute environment at high concentration (22% H) in a silicon complex of radius 6.0 Å. (b) A silicon complex consisting of 19 H atoms in a radius of 6.0 Å at high concentration. Several (four–seven) hydrogen atom clusters are visible in the complex. Silicon and hydrogen atoms are indicated in green (large) and yellow (small), respectively.

with results from NMR studies [13, 14]. The size of the clusters varies from 5.0 to 7.0 Å, and one such cluster is identified and presented in figure 5(b). It may be noted that at low concentration all the dihydride configurations are realized in a clustered environment, indicating the absence of isolated dihydrides in the model.

At high concentration (22% H), the microstructure is mostly dominated by clusters rather than a dilute or sparse distribution of hydrogen. A real-space analysis of the 611-atom model reveals the presence of some large clusters in the network. An example of such a cluster that consists of as many as 19 H atoms in a complex of radius 6.0 Å is shown in figure 6(a). These clusters mostly consist of silicon monohydrides (SiH) and dihydrides (SiH$_2$), but a few SiH$_4$ configurations are also found in our model [28]. While the microstructure at high concentration is dominated by the presence of clusters, a few monohydrides persist in a very dilute or isolated environment. In figure 6(b) we have shown two such lone monohydrides that are found in a silicon complex of radius 6.0 Å.

An important aspect of the microstructure at high concentration is the presence of several SiH chains in the network. Some monohydrides can form an open chain-like structure at high concentration via bond formation between the Si atom in the monohydrides. The chain structure that we have observed consists of four–seven monohydrides (SiH). A few structures are also observed where monohydrides in the chain are replaced by dihydrides. Examples of such chain-like structures are shown in figure 7. The structure on the left (of figure 7) consists of six monohydrides (SiH) that are connected via Si–Si bonding, whereas the structure on the right has four monohydrides and a single dihydride. Such chain configurations are not observed in the model with low concentration (7%) of hydrogen. It should be noted that the presence of such chain-like structures was reported by Lucovsky et al [20], Manfredotti et al [18] and Baum et al [14] in their IR and NMR experiments, respectively.

5. NMR widths from the Van Vleck moments: an approximate calculation

Although a direct determination of the width and the shape of the NMR spectrum for amorphous solids is highly nontrivial,
Figure 7. The formation of open chain-like structures via Si–Si bonding at high concentration (22% H). The structure on the left is comprised of seven monohydrides connected via silicon atoms to form an open chain. The structure on the right shows four monohydrides and a single dihydride. As before, silicon and hydrogen atoms are indicated in green (large) and yellow (small), respectively.

an approximate value for the same can be obtained from the knowledge of the Van Vleck moments of the resonance spectrum. Since the contribution to the higher moments generally comes from the wings of the spectrum and is difficult to observe in experiments, the first two or three non-zero moments should suffice to capture the main features of the resonance curve [38]. It should, however, be noted that a one-dimensional NMR spectrum cannot fully represent every aspect of a three-dimensional spin (hydrogen) distribution in real space, and further information is needed for a complete description of the latter. Following Van Vleck [33], the second and the fourth moments of a system of \( N \) particles (of spin 1/2) can be written as

\[
\frac{M_2}{\gamma \hbar^2} = \frac{1}{2N} \sum_{j<k} B_{jk}^2,
\]

\[
\frac{M_4}{\gamma \hbar^4} = \frac{3}{16N} \sum_{(jkl)} B_{jk}^2 B_{jl}^2 - \frac{1}{36N} \sum_{(jkl)} B_{jk}^2 (B_{jl} - B_{kl})^2
\]

\[+ \frac{1}{72N} \sum_{(jkl)} B_{jk} B_{kl} (B_{jl} - B_{jk}) (B_{jl} - B_{kl}) \]

\[+ \frac{1}{8N} \sum_{j<k} B_{jk}^4,
\]

where

\[
B_{ij} = \frac{3}{2} \left( 1 - 3 \cos^2 \theta_{ij} \right) \frac{1}{r_{ij}^3}
\]

and the symbol \( (jkl) \) stands for no two indices being equal in the triple sum\(^2\). The shape and the width of the resonance curve can be interpreted in terms of the second and the fourth moments. For an ideal Gaussian, \( \Gamma = M_2/M_4^2 = 3 \), and the full width at half maximum (FWHM) is given by \( \sqrt{8M_2 \ln 2} \). A small value of \( \Gamma \) indicates a bi-modal nature of the spectrum. On the other hand, at low concentration and in a dilute environment, a truncated Lorentzian is a useful approximation. The FWHM in this case is given by \( \sigma = \sqrt{\frac{2\pi}{3\Gamma}} \). In practice, the experimental curve can deviate significantly from the Gaussian or a truncated Lorentzian behavior depending on hydrogen concentration, preparation conditions and the degree of inhomogeneity present in the samples. For a small deviation, one often uses the Gaussian memory function approximation and expresses the universal line width as [39]

\[
\sigma_u = \sqrt{\frac{2\pi}{\Gamma - 2}} \quad \text{for } \Gamma > 3. \tag{3}
\]

Since the experimental values of the width are obtained by deconvoluting a resonance spectrum into a broad (typically Gaussian) and a narrow (a truncated Lorentzian) part, it is important to take into account this fact while calculating the corresponding theoretical values. This is particularly important for the calculation based on models of limited size in the presence of strong inhomogeneities in hydrogen distribution. For example, the presence of a single large cluster in the

\(^2\) It may be noted that the analytical expression for the fourth moment given in [38] cannot be employed to calculate the same for an arbitrary distribution of spins in a disordered network. The expression is valid only for crystalline lattices at high concentration of spins.
network at low concentration can dominate the moment sums in equations (1) and (2). The effect of the dilute environment can be missed out in this case, and may not be reflected in the calculated values of the narrow width via the Lorentzian approximation. In the present work, we have avoided this by partitioning the overall microstructure into two regions consisting of clustered and dilute phases. The moments from the corresponding regions are then employed for the calculation of the widths of the broad and the narrow part of the spectrum, respectively. This partition of the spins into clustered and dilute regions in real space can be viewed as analogous to the deconvolution of a one-dimensional NMR spectrum into a broad and a narrow part. In the following, we discuss the results for the NMR line widths obtained for two different concentrations by partitioning the microstructure as stated above.

The broad and the narrow line widths of the NMR spectra for the models with two different concentrations are listed in Table 1. As mentioned earlier, the broad line width is calculated via equation (3) using the moments from the clustered region. Similarly, the narrow line width can be obtained from the moments for the dilute region via the Lorentzian approximation. In addition to these, we have also listed the value of the narrow line width estimated from the density of hydrogen atoms (n) in the dilute region using \( \sigma_{narrow} = 4\pi\gamma^2\hbar\sqrt{n}/(3\sqrt{3}) \) [38]. Since the latter is often used by experimentalists to get an approximated value of the narrow line width, this provides a quick way of comparing our results to the experimental data.

The NMR experiments of Reimer et al [13] and Gleason et al [12] indicated that the broad line width typically lay in the range from 22 to 30 kHz, whereas the narrow line width was of the order of 3–5 kHz for typical device-quality samples with 8–15% hydrogen concentration. A similar observation was also noted in the NMR experiments of Carlos et al [17] with a 20% variation of line width. These results are comparable to the values of 19.0–25.0 kHz obtained from our model with 7% H. The calculated value of the broad line width for the model with 22% H is found to be somewhat larger than the experimental value. However, this can be explained by taking into account the presence of a large cluster in the model (cf figure 6(a)). The presence of such a large cluster is not surprising and has been reported by Wu et al [15], who observed a broad line width in hot-filament-assisted chemical vapour deposited films. These authors have observed a new hydrogen distribution with a line width as broad as 47–53 kHz for the hot wire (HW) samples of concentration 2–3% H. This implies that even at very low concentration it is possible to have a few large clusters of hydrogen in the samples that can produce a line width as broad as 50.0 kHz. The presence of such inhomogeneities warrants the need for partitioning the network into two regions for the calculation of the narrow line width.

6. Conclusion

The distribution of hydrogen atoms in amorphous silicon is studied at low and high concentrations (of hydrogen) with particular emphasis on the presence of mono- and divacancies. A remarkable feature of the microstructure is the presence of mono- and divacancies both at low and high concentrations. These vacancies are realized in the models as a ‘built-in’ feature and are not incorporated or introduced by hand as in most of the previous studies. The presence of such vacancies has been observed using IR absorption spectroscopy on hydrogenated amorphous silicon samples obtained via expanding thermal plasma techniques. The widths of the NMR spectra of the model networks are calculated using the second and the fourth Van Vleck moment of the spectrum by partitioning the microstructure in real space into a dilute and a clustered region. The values of the line width obtained in this work are in excellent agreement with experimental data from the NMR and the multiple-quantum NMR studies. Our results suggest that for highly inhomogeneous distribution of H in the network, the width and the shape of the NMR spectrum is significantly influenced by the fourth moment. Hydrogen atoms are found to be distributed in a dilute or sparse environment and a dense or clustered environment in the silicon matrix. At low concentration, the microstructure is characterized by the presence of a few small clusters in the background of a sparse distribution of hydrogen. On the other hand, the microstructure is found to be strongly inhomogeneous at high concentrations that consist of a few large and several small clusters along with a few chain-like structures. These observations are consistent and supported by multiple-quantum NMR and IR spectroscopic data.

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| Observations | Concentration (% H) | NMR line widths |
|--------------|---------------------|-----------------|
| Present work | 7.0                 | Narrow 4.9–5.3  |
|              | 22.0                | Broad 5.9–9.6. |
| Experiments  |                     |                 |
| Reimer et al | 8.0–32.0            | Narrow 3.0–5.0  |
| Gleason et al| 8.0–15.0            | Broad 22.0–27.0 |
| Wu et al     | 8.0–10.0            |                 |
| Wu et al     | 2.0–3.0             |                 |

Table 1. Experimental and theoretical values of the NMR line widths.
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