Generation of a large structure (10^5 atoms) of amorphous Si using molecular dynamics

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Abstract. A method for generating amorphous tetrahedral structures having 13 824 and 110 592 atoms is presented. We took the Wooten, Winer and Weaire amorphous model of 216 atoms and put together a number of these blocks. This larger structure was annealed using molecular dynamics and then cooled. Comparison with experiment was carried out using the structure factors calculated directly. Very good agreement has been attained. The generated structures, contrary to the original WWW model, contain coordination defects.

1. Introduction

The very first problem when dealing with amorphous materials, is their structure and how to describe the atomic order in such materials. Because of a lack of the long range order (LRO) or periodicity, the standard methods of crystallography fail in this case. Short range order (SRO) in amorphous material is usually described using the radial distribution function (RDF). This function can be easily derived for any model but there are many difficulties when the model is small and periodic boundary conditions (PBC) are applied.

If any model of an amorphous system is constructed the next step is to compare it with experimental data. Information about the atomic structure factor in a disordered system is usually obtained using x-ray or neutron scattering. In order to derive the RDF from these data one has to carry out an additional data manipulation which is far from being straightforward because of the limited range of q values and the limited experimental resolution (for the discussion of this point see, for example, Etherington *et al* 1982). On the other hand, the experimental scattering curves correspond directly to the structure factor $S(q)$. The structure factor can be directly calculated for a model provided one has a model of sufficient size (we will return to this point in section 4).

In this paper we have constructed a very large model of an amorphous tetrahedral material (silicon or germanium) using molecular dynamics. Instead of verifying it using the RDF, as is done usually, we have calculated the structure factor directly and compared it with very recent experimental data. In this way we avoided a lot of problems with the RDF calculation and with ambiguities related to obtaining the RDF from experimental data.

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We compared the model for $S(q)$ with scattering results for Si (Fortner and Lannin 1989). The preliminary results of our studies have already been published (Holender and Morgan 1991) but this paper represents a further advance using an improved algorithm and a much larger number of atoms. Also, a more detailed analysis is carried out.

2. Interatomic potential

It is now well established that pair potentials alone are unable to describe tetrahedral semiconductors. The situation can be improved with a first principles technique (Car and Parrinello 1985) or by using phenomenological potentials (an up-to-date review on this problem can be found in Carlsson 1990). There are also some intermediate approaches, for example the empirical tight-binding molecular dynamics (ETBMD) of Wang *et al* (1989), Khan and Broughton (1989) or Laasonen and Nieminen (1990).

First principle methods are very attractive and have already been applied to amorphous silicon, for example Car and Parrinello (1988) or Drabold *et al* (1990) but they are extremely computationally demanding so that, at present, they can be applied to only very small systems (less than 100 atoms). If, however one is going to simulate bigger systems (more than 1000 atoms) one must, at current computational capabilities, apply phenomenological potentials. However, there is the very recent paper on ETBMD simulations of 512 atoms of Si by Wang *et al* (1991).

In phenomenological approaches the 'cluster potentials' (e.g. Stillinger and Weber 1985, Pearson *et al* 1984, Biswas and Hamann 1987) or the 'cluster functionals' (Tersoff 1988, Baskes 1987, Bolding and Andersen 1990) are used. Some potentials have been applied successfully to the various simulations of a-Si. The Stillinger and Weber (1985) potential was used by Kluge *et al* (1987), Broughton and Li (1987), Luedtke and Landmann (1988, 1989a, b), and very recently by Kwon *et al* (1991) for studies of Staebler–Wronsky effect in a-Si, and by Ding and Andersen (1986) for amorphous germanium. The Biswas and Hamann (1987) potential was used by Biswas *et al* (1987). The Stillinger and Weber (1985) potential was also used for binary amorphous systems such as Mo–Ge (Ding and Andersen 1987) and Si–H (Mousseau and Lewis 1990, 1991).

There are many papers comparing various potentials and analysing their applicability. The general validity of the Stillinger and Weber (1985) potential is not completely clear. Cowley (1988) for example, concluded that the potential gives the best overall description of Si. Kluge *et al* (1986) found however, that it does not describe elastic properties correctly. It also fails to describe some surface properties of Si (e.g. Wilson *et al* 1990). On the other hand there are many papers supporting the application to amorphous silicon and germanium, usually with increased strength of the three-body component of the potential compared with the original value.

We decided to use the Stillinger and Weber (1985) potential. This potential is composed of a standard pair term and an additional three-body component stabilizing the tetrahedral network of silicon. We carried out, however, the additional simulations using an increased value for the three-body strength following the papers of Ding and Andersen (1986), Biswas *et al* (1987), Broughton and Li (1987) and Luedtke and Landman (1988). For the parameter λ we used value 31 (for the Stillinger and Weber 1985 potential $\lambda = 21$). This potential corresponds exactly to that derived by Diang and

Andersen (1986) for Ge except for energy and length scaling. We will denote this modified potential by SWM. This modification decreases the probability of large deviations from tetrahedral structure. The original Stillinger and Weber (1985) potential was aimed at describing correctly the liquid and solid phases. Ding and Andersen (1986) suggested that there are no parameters which describe, simultaneously, all three phases (solid, liquid, and amorphous) correctly. They reported that a correct description of solid and amorphous germanium can be attained with an increased strength for the three-body potential. On the other hand, Luedtke and Landmann (1989a), in their later paper, insisted that it is only a matter of sufficiently long simulations and that the original Stillinger and Weber (1985) values work for a-Si.

3. Method of a-Si generation

The generation of the amorphous structures has been performed in various ways starting from the first principles methods discussed in section 2. A common feature of these first principle models is the small size of the amorphous block of material. For Car and Parrinello (1988) and Drabold *et al* (1990) the number of atoms in a cubic cell was 54 and 63 respectively.

Wooten *et al* (1985) constructed an amorphous tetrahedral network (denoted by WWW) composing 216 atoms by starting from a crystalline material and performing stochastic atomic rearrangements. This model, composing 216 atoms, has a periodicity in the x, y, and z directions equal only to three lattice constants of c-Si namely 16.29 Å.

The most usual method for generating a-Si is to melt Si using molecular dynamics (MD) and quench or cool it. This technique was applied by Car and Parrinello (1988), Drabold *et al* (1990), Kluge *et al* (1987), Biswas *et al* (1987), Broughton and Li (1987), Luedtke and Landmann (1988, 1989a) and by Ding and Andersen (1986) for amorphous germanium. These models usually contain hundreds of atoms. Luedtke and Landmann (1989b) obtained a-Si by simulating atomic deposition.

In order to reduce the amount of the computer time required for the amorphization of the structure and to avoid problems with obtaining a-Si by quenching a liquid we used the WWW structure as a starting point. We first relaxed this structure using the Stillinger and Weber (1985) potential. Only small displacements took place but the size of the box changed slightly so that the equilibrium density ρ of the block is 0.958 of that for crystalline silicon. For the original WWW model the minimum in-total energy is reached for $\rho = 0.949$, see figure 1 (dotted curve). If we relaxed the WWW structure (we will denote this relaxed structure as WWWR) for a sufficiently long time the structure has a minimum at $\rho = 0.958$ and the energy is slightly (0.5%) lower (dashed curve in figure 1). The corresponding curve for crystalline silicon (solid curve) is shown for comparison. The analogous plots for the Stillinger and Weber (1985) modified potential (SWM), with $\lambda = 31$ instead of 21, are shown in figure 2.

The WWWR structure was used in subsequent calculations. At first we put together eight such blocks forming a system of 1728 atoms, twice as large in any direction. We heated it in order to get rid of an old periodicity (we applied 3D PBC for this larger system but the periodicity in any direction was initially two times smaller than the actual block size). After cooling this larger amorphous block we repeated this procedure to obtain the amorphous model containing 13 824 atoms and once more for a model of 110 592 atoms. The later model created an upper limit of our computational abilities.
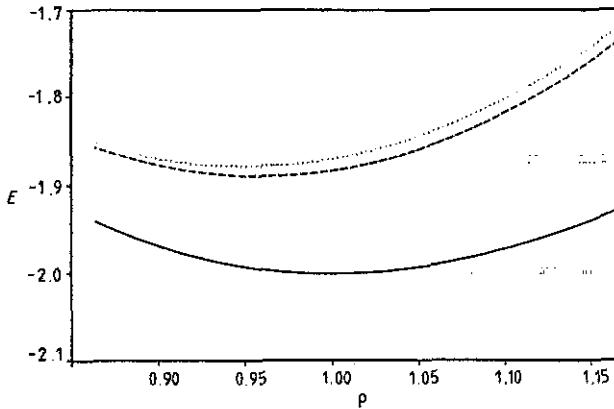
Figure 1. Energy versus density curves for the Stillinger and Weber (1985) potential for the WWW structure (dotted curve), relaxed WWWR structure (dashed curve) and crystalline Si (solid curve). Energy is expressed in Stillinger and Weber (1985) units (2.17 eV atom^{-1}) and ρ is expressed in the density of c-Si unit.

4. Structure factor calculations

Because of the reasons given in the Introduction we decided to calculate the structure factor directly and not via Fourier transformation of the RDF as is usually done. We directly evaluated the sum

$$S(q) = \frac{1}{N} \sum_n \exp(iq \cdot R_n) \sum_n \exp(-iq \cdot R_n)$$

where R_n denotes the position of the nth atom and N the total number of atoms.

This quantity was calculated by a direct summation for a set of q_x, q_y and q_z chosen according to the periodic boundary conditions, i.e. $q_x = n_x 2\pi/L$, $q_y = n_y 2\pi/L$, and $q_z = n_z 2\pi/L$ where L is a size of the box and n_x, n_y, n_z are integers. Because we are dealing with a system which is isotropic on a macroscopic scale we calculated S as a function of the modulus q by averaging over all orientations. The fluctuations in $S(q)$ provided us with a perfect test for the disappearance of the internal periodicity. If we put together some blocks we increase the number of available q point but as long as any additional periodicity remains the values of $S(q)$ at these additional points is equal (or close) to zero. Calculated in this way $S(q)$ contains, as is obvious, a lot of 'noise' corresponding to interference between waves from atoms separated by large distances. Experimental curves are smooth because of limited resolution but in reality contain very rapid fluctuations which are not measurable. Finally, in order to compare with experiment all our $S(q)$ curves were convoluted with a Gaussian. Its width depends on the size of system (see section 6). We used a Gaussian with a standard deviation $\sigma = 0.05$ Å^{-1} for 13 824 atoms while for 110 592 atoms we used $\sigma = 0.025$ Å^{-1}. The multiplicity of various values of q was taken into account all the time. It is essential for such simulations to have a sufficiently large model (over 1000 atoms) because the size of the model determines the density of available points in q space. It can be a severe restriction at low values of q if the box is small.
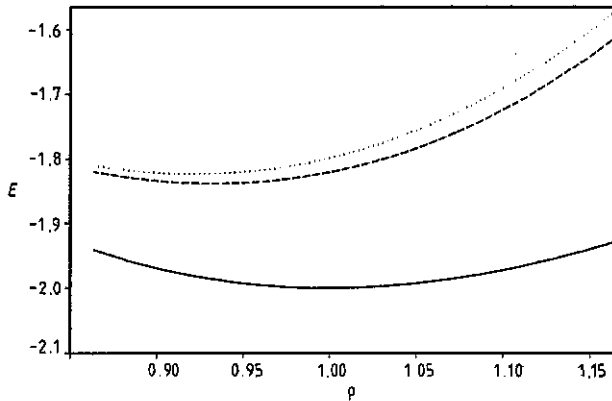
Figure 2. The same as in figure 1, for the SWM potential.
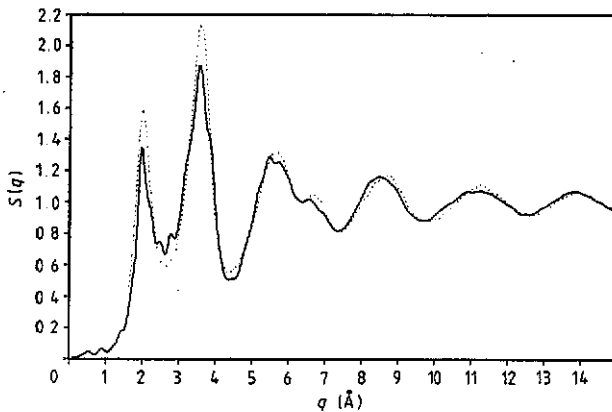
Figure 3. The comparison of $S(q)$ for our model M1 (solid curve) with results obtained by Fortner and Lannin (1989) (dotted curve) for a film 'annealed at 600 °C for 1 h'.

This method for calculating the structure factor was applied by Guttman (1981) in his studies of the hydrogenated silicon but because of small number of atoms he was unable to get accurate curves for small values of q.

5. Molecular dynamics method and the 'thermal treatment'

A standard Molecular Dynamics (MD) technique was used with Andersen's (1980) method of constant pressure. The iteration time was equal 1.5×10^{-15} s and the standard 'leap-frog' algorithm was used. The temperature was kept constant by scaling the velocities at every iteration step, which can be thought of as a reasonable approximation to a canonical ensemble (e.g. Nose 1990).

The optimum thermal treatment we were looking for was not intended to resemble the real experimental generation of a-Si. Rather, we were looking for the most efficient method for the computer generation of a model of a–Si with large dimensions. The final
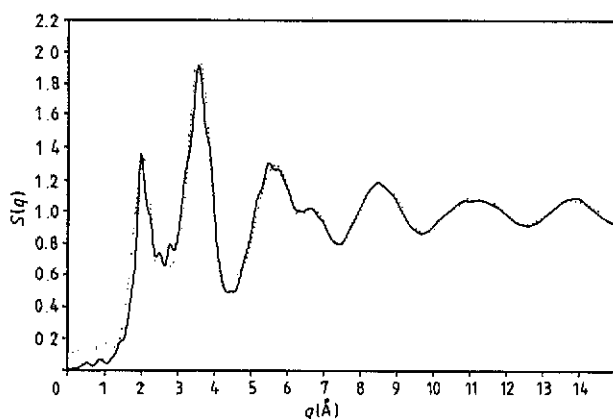
Figure 4. The comparison of $S(q)$ for our model M1 (solid curve) with that obtained by Etherington *et al* (1982) for Ge and scaled to represent Si (dotted curve).

Table 1. The characteristics of our models M1 and M2 and that of the Landman and Luedtke (LL) model (1989a).

	M1 0 K	M2 0 K	M1 RT	M2 RT	LL RT
ρ	0.995	0.943	0.993	0.940	1.006
R_{min}	2.93	3.04	2.93	2.99	2.87
N_3	0.05%	2.0%	0%	2.18%	0%
N_4	73.9%	93.5%	73.6%	93.74	78%
N_5	24.8%	4.5%	24.6%	4.04%	21%
N_6	1.2%	0.01%	1.5%	0.01%	0.02%
N_{av}	4.28	4.03	4.28	4.02	4.21
E_{tot}	−1.90	−1.83	−1.88	−1.81	−1.89
E_2	−2.14	−1.98	−2.14	−1.97	−2.13
E_3	0.24	0.15	0.26	0.16	0.24

RT—room temperature; ρ—density (1 for c-Si); R_{min}—position of the first minima in RDF (in Å); N_i—percentage of i-coordinated atoms, coordination is defined by R_{min}; N_{av}—average number of NN; E_{tot}—total energy in (ε units); E_2, E_3—two and three body contributions to total energy.

criteria of acceptance for the structure was the degree of agreement with experimental structure factors.

At first we applied the trial and error method for heating our systems. At this point we had to find some criteria as to which structure should be accepted or rejected. While increasing the periodicity of the model we must introduce some disorder but we have to prevent the structure from melting because of the well-known problem of generating a–Si from the melt.

The following criteria was used. The first is the structure factor itself. If we increase the size of the system by two we increase the number of available q points but as long as additional periodicity remains the values of $S(q)$ at these additional points is equal (or close) to zero and at the remaining points is eight times higher (the average value is the
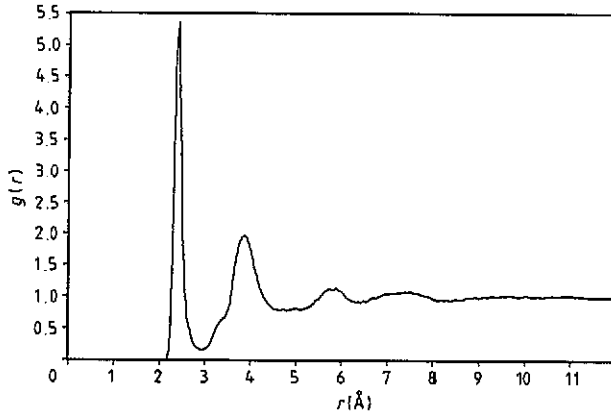
Figure 5. The radial distribution function for our model M1 (for $r > 12$ Å it is very close to unity).
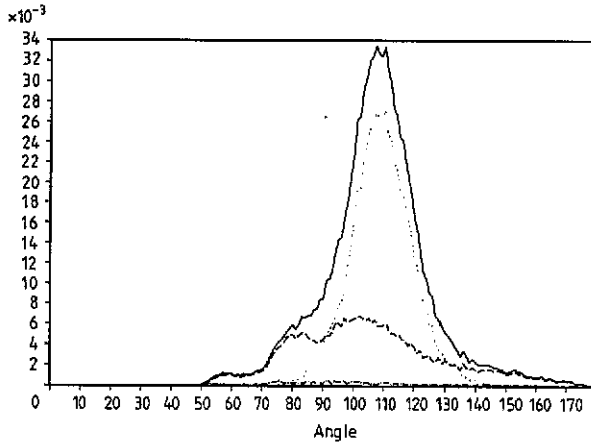

Figure 6. Bond angle distributions for model M1—the total distribution (——) and partial distributions corresponding to atoms having four ($\cdots$), five (– – –) or six (–·–·) nearest neighbours.

same). Our heating procedure resulted in a structure factor which for $q > 5$ Å^{-1} was greater than 0.6 and smaller than 1.4 for the vast majority of points in q-space and clearly indicates that the additional periodicity has been destroyed.

On the other hand we must not melt the sample. If the sample melts the density and coordination increase and an additional peak appears in the RDF on the shoulder of the second peak (e.g. Broughton and Li 1987). It is extremely difficult to remain to the amorphous state from this over-coordinated liquid.

6. Results

After many tests we generated structures in the following way. We heated the sample for 2500 iterations at 1000 K (this is below the melting point of the Stillinger and Weber
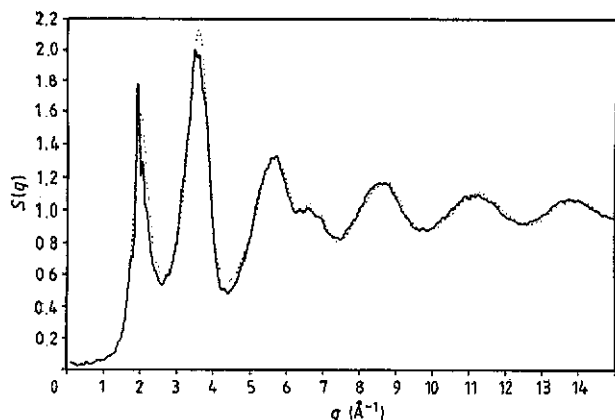
Figure 7. The comparison of $S(q)$ for our model M2 (solid curve) with results obtained by Fortner and Lannin (1989) (dotted curve) for a film 'annealed at 600 °C for 1 h'.
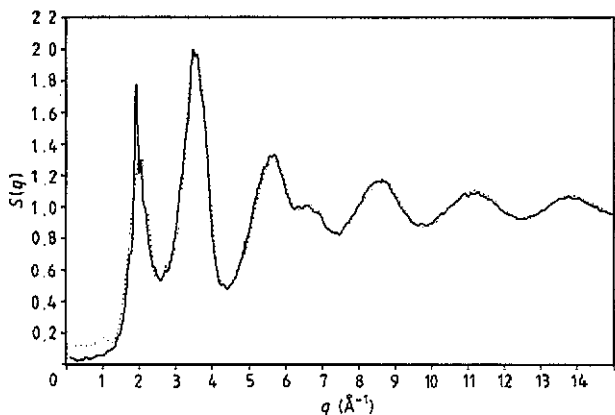

Figure 8. The comparison of $S(q)$ for our model M2 (solid curve) with that obtained by Etherington *et al* (1982) for Ge and scaled to represent Si (dotted curve).

(1985) c–Si but about the melting point of the Stillinger and Weber (1983) www structure) and cooled it down to 0 K during the next 1000 iterations. The structure was later kept at 0 K until further atom re-arrangements were negligible. Later it was equilibrated at room temperature (300 K) in order to enable comparisons with the experiments carried out at room temperature. The structures at 0 K and at room temperature are almost identical. The results for the original Stillinger and Weber (1985) potential and 13 824 atoms (model denoted by M1) are shown in figures 3–6 and in table 1. The bond angles distributions are obtained by calculating the angles formed by any atom and its nearest neighbours (NN). The NN are defined by R_{min} the first minimum in the RDF (see table 1). The partial distributions were obtained by analysing central atoms having a specified number of NN. We used two sources of the experimental $S(q)$ curves in our study. One source is the result for Si obtained recently by Fortner and Lannin (1989) (in order to make plots clearer we took only the results for the sample annealed at elevated temperature) and the second source is data for Ge obtained by Etherington *et al* (1982).
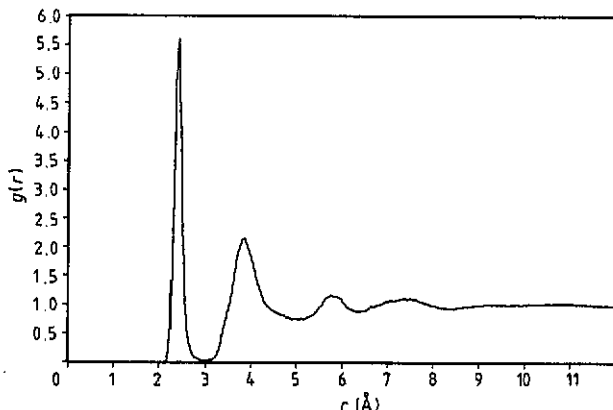
Figure 9. The radial distribution function for our model M2 (for $r > 12$ Å it is very close to unity).
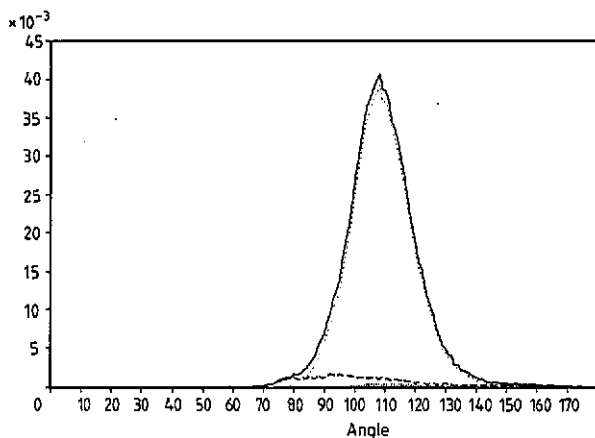
Figure 10. Bond angle distributions for model M2—the total (——) distribution and partial distributions corresponding to atom having three ($\cdots$), four ($\cdot\ \cdot\ \cdot$), or five (– – –) nearest neighbours.

This data is rescaled from Ge to Si so this comparison can be also regarded as a test of the potential for a-Ge with a rescaled length unit.

For the potential SWM (model M2) the treatment was the same except for the annealing temperature. In this case we had to heat at 2500 K in order to remove the old periodicity. This results are shown in figures 7–10 (for 13 824 atoms). In figure 11 we show the unsmoothed curve for the model M2, and the rapid fluctuation mentioned in section 4 can be clearly seen. That such fluctuations must exist is easily shown by evaluating the root mean square of the structure factor. If, for simplicity, one takes a random system it is easily shown that the fluctuations are of the same order as the structure factor itself.

The structure factors for the model M2 composed of 110 592 atoms are shown in figure 12. All the other features (energy, density, percentage of defects) of this model
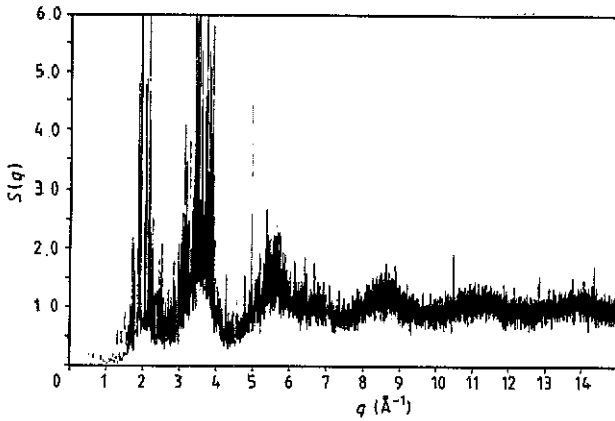
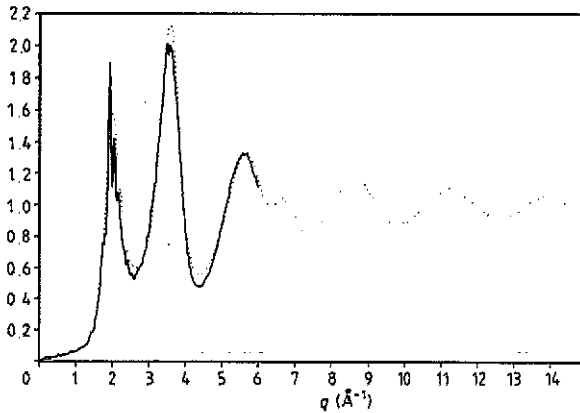**Figure 11.** Unsmoothed structure factor for the M2 model.

Figure 12. Structure factor for model M2 composed of 110 592 atoms (solid curve) compared with that obtained by Fortner and Lannin (1989) (dotted curve) for a film 'annealed at 600 °C for 1 h'.

are almost the same as for the model M2 composed of 13 824 atoms. For the larger system we were able to use a narrower Gaussian. The structure factors obtained for various model sizes and using different widths for the Gaussian are shown in figure 13. If we increase the dimensions of a system by a factor of two (eight times more atoms) we can halve the width of the smoothing Gaussian. The quality of curves is more or less the same but for the bigger system fine details in $S(q)$ are visible (for example splitting of the first peak in figure 12). We are not able to verify all the details of $S(q)$ experimentally because the 'resolution' we can obtain in our simulations is higher than the experimental one. The comparison with experiments should be carried out using mainly the second and further peaks because the amplitude of the first peak is very sensitive to the applied smoothing and this is probably true for experimental results as well. The amplitudes and shapes of the remaining peaks are almost independent of the Gaussian width (see figure 13).
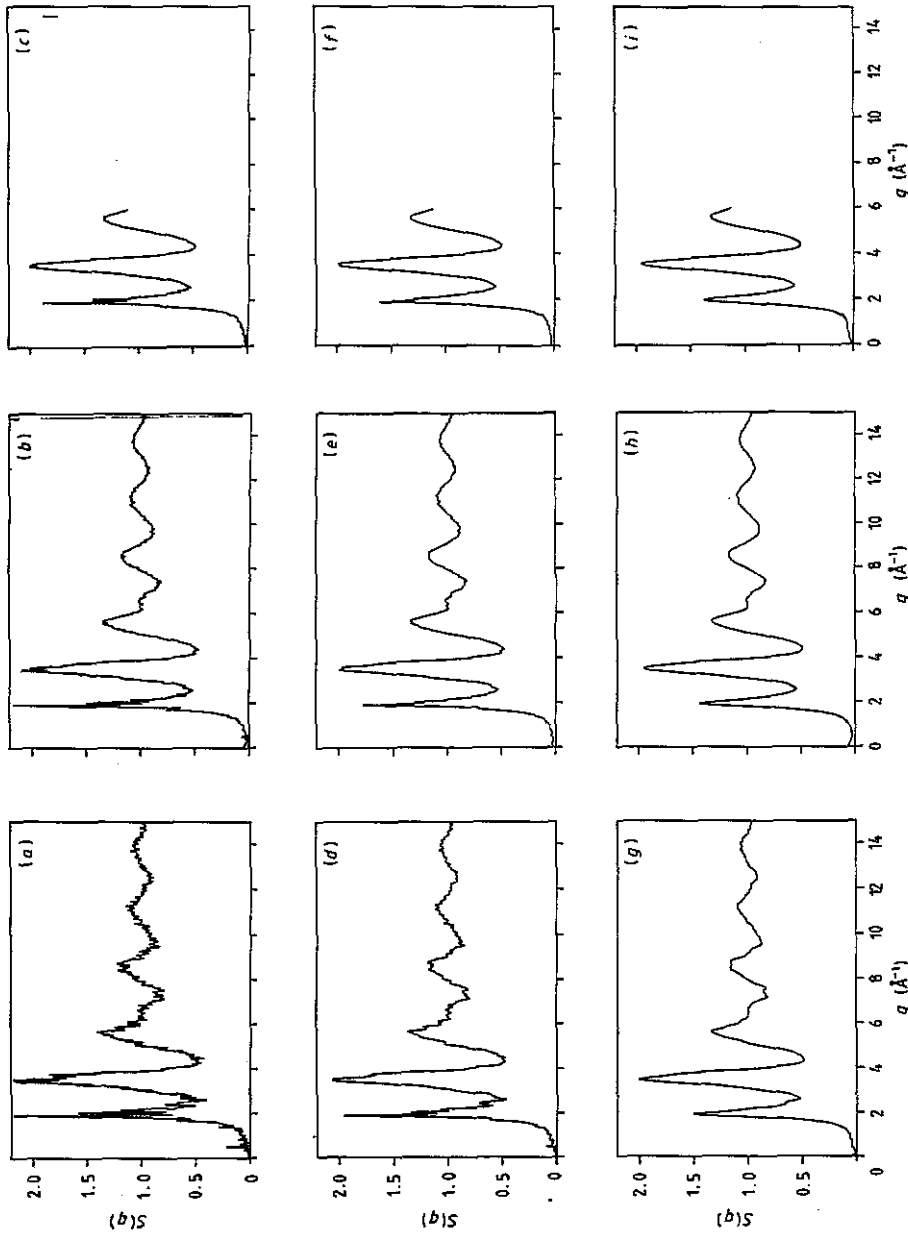
Figure 13. The comparison of structure factors for various number of atoms N and various width σ of the Gaussian smoothing function: (a) $N = 1728$, $\sigma = 0.025\,\text{Å}^{-1}$; (b) $N = 13\,824$, $\sigma = 0.025\,\text{Å}^{-1}$; (c) $N = 110\,592$, $\sigma = 0.025\,\text{Å}^{-1}$; (d) $N = 110\,592$, $\sigma = 0.05\,\text{Å}^{-1}$; (e) $N = 1728$, $\sigma = 0.05\,\text{Å}^{-1}$; (f) $N = 110\,592$, $\sigma = 0.05\,\text{Å}^{-1}$; (g) $N = 1728$, $\sigma = 0.05\,\text{Å}^{-1}$; (h) $N = 13\,824$, $\sigma = 0.1\,\text{Å}^{-1}$; (i) $N = 110\,592$, $\sigma = 0.1\,\text{Å}^{-1}$.

The density of the M1 model is almost exactly equal to the density of c-Si. For M2 the density was lower (0.943 of the density of c-Si). This is very close to the experimental value 0.955 reported by Fortner and Lannin (1989). Our models M1 and M2 also differ in the number of the coordination defects. Here coordination is defined by the number of neighbours closer to an atom than the first minimum in the RDF (R_{min}, see table 1). This seems to be a reasonable definition of nearest neighbours, and the overall number of coordination defects is not very sensitive to the choice of R_{min} in the range close to the minimum in the RDF. From a detailed analysis of the structure using 3D graphics, we can conclude that the coordination defects are real and that we cannot remove a defect by small displacements of atoms. For the M2 model, defects are distributed quite randomly in the system and very often three or five coordinated atoms are surrounded only by four coordinated atoms.

The M1 model gives a high number of coordination defects. It is a feature of the Stillinger and Weber (1985) potential, and all a-Si models generated using this potential have a high percentage of over-coordinated atoms. On the other hand the M2 model gives a more reasonable concentration of 'defects'. The $S(q)$ form and density also seem to be closer to experimental values. The experimental and model $S(q)$ curves differ slightly in the form of the first peak but, as discussed above, it may be the effect of the smoothing we applied.

The total bond angle distribution for M1 is peaked at the tetrahedral angle but there is a well marked distortion on the small angle shoulder. The partial curves clearly show that this distortion is due, almost entirely, to five coordinated atoms.

It is worth noticing that the shape of these curves is almost identical with ones obtained by Luedtke and Landman (1989a). The quantitative comparison is slightly complicated because they normalized every curve independently so information about relative intensities is lost. The percentage of three, four and five coordinated atoms are also very close to our results (see table 1). We have therefore generated structures with features which are, in general, similar to those of the Landman and Luedtke model (1989a) but of course our structures are much larger (they had only 588 atoms). They created their model by slow cooling from the melt and needed about 3×10^6 iteration steps to generate the structure while we are able to obtain a very similar structure in less than 10^4 iterations. This is a great advantage in starting from the WWW model.

The corresponding total bond angle distribution for the M2 model (figure 9) is dominated by four coordinated atoms and so there is almost no distortion.

7. Discussion and conclusions

The importance of good a-Si (or a-Ge) models for theoretical considerations is quite obvious. It is extremely useful, from a theoretical point of view, to have big 'ideal' structures without some of the features inevitably induced by particular methods of preparation. The fine details in $S(q)$ are very important in calculating electron properties of a-Si (Morgan *et al* 1989). The larger structures also create opportunities for studying defects, transport properties and so on. In this paper we took advantage of the WWW model as a very good approximation of a-Si for a small number of atoms. By starting from the WWW model we saved a lot of computer time. Our model after scaling can also be treated as a model of a-Ge. For all models we applied 3D PBC. The periodicities for the M2 model of 13 824 atoms and 110 592 atoms were about 66.4 Å and 132.8 Å respectively.

There are some features which distinguish our model from WWW. The very first is the fact that we have coordination defects. The concentration for M1 seems to be to high (it seems to be an unavoidable feature of the Stillinger and Weber (1985) potential). For M2 the number of defects is much more reasonable but it is not clear if this is representative of a real system.

We can conclude that the modified Stillinger and Weber (1985) potential with a higher value of three-body contribution ($\lambda = 31$ instead of 21) is more suitable for the amorphous system. This potential will not work correctly for the liquid state and will not predict a correct value for the melting point. It has already been claimed by Ding and Andersen (1986) that there are no parameters for the Stillinger and Weber (1985) potentials which work simultaneously for all condensed phases.

We have verified our model using directly calculated $S(q)$ curves instead of the RDF. This approach seems to have many advantages but there are some limitations. One has to have a model of relatively large size (over 1000 atoms at least) otherwise the density of points in q space is too small especially for low values of q.

There is, however, no unique relation between the real space structure and structure factor. Agreement between structure factors does not necessarily mean that the real space structures are identical. Our model M2 does however seem to be in close agreement with available experimental data.

We should also comment on the computational effort for evaluating $S(q)$. It increases dramatically with the size of a model. If we increase the box size m times the number of atoms is increased by m^3 and the number of points in q space increases also as m^3 so the time of the calculations increases as m^6.

We are now in the process of applying our model to calculate the electronic properties of a-Si. The structures generated in this paper will be also used as a basis for further studies of the properties of hydrogenated a-Si.

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