Radial distribution functions and local densities in simulated thin polymeric films near the glass transition

Student: Koen Weerts
Supervisors: Prof. dr A.R.C. Baljon
Dr A.V. Lyulin

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Abstract

In this report, the glass transition of a thin polymer film is studied. In the film, there are 40 polymer chains, each containing 100 beads. The interactions in the film are described with the Lennard-Jones potential, and the FENE-potential. There are already three methods to calculate the glass transition temperature. The first method uses the film thickness. The glass transition obtained with this method is $T=0.51$. The second method makes use of the heat capacity. The maximum of the heat capacity is taken as the glass transition temperature. This maximum is $T=0.5$. The third method is diffusion, with a glass transition temperature of $T=0.36$. These results are obtained for ungrafted films.

A fourth method uses the radial distribution function. The radial distribution function is calculated for different temperatures. The inverse maximum of the first and second peak of the radial distribution function are plotted against temperature. At the glass transition temperature, the slope of these curves changes.

The radial distribution function is calculated for different films. One of the films is grafted the other is ungrafted. The peaks for the grafted films are higher than the peaks for the ungrafted films.

In the lower half of the film, a difference is made between immobile particles and the other particles. The radial distribution function is calculated for the immobile particles and the rest. The peak of this function is higher for the immobile beads.

The thin film is divided in 14 layers. In each layer the radial distribution function is calculated, and the height of the peak is plotted in function of the layer. The further from the substrate, the lower the peak, the lower the local density.

As a last thing, the scattering function, the Fourier transform of the radial distribution function, is calculated. Again the inverse maximum of the scattering function is plotted against temperature.
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1. Introduction

Glass transition occurs due to a reduction in motion of large segments of polymer chains with decreasing temperature. Upon cooling, a liquid of long and/or cross-linked polymers changes into a liquid-like material; the glass transition corresponds to the gradual transformation from a rubbery material into a rigid solid-like material. The glass transition temperature is the temperature at which the polymer melt changes from a rubbery state into a solid-like state or vice versa. In addition, abrupt changes in other physical properties accompany this glass transition.

In our simulation, 40 polymer chains, each containing 100 monomers are used. The thickness of the film is almost 14σ. σ is the length scale of the LJ-potential and was between 0.4-1 nm. The film is divided in 14 layers. The first layer has a thickness of 1.45σ, the others a thickness of 0.9σ (figure 5).

There are already three methods used to calculate the glass transition temperature [1]. These make use of the film thickness, the heat capacity and the diffusion. In the first method, the film thickness is studied as a function of the temperature. The film thickness for liquid and the glassy parts are both linear related functions to the temperature. The point of intersection of those two parts is defined as the glass transition temperature.

![Figure 1: Film thickness as a function of temperature for the ungrafted film. \( \varepsilon_{\text{ps}} = 1 \), \( \varepsilon_{\text{ps}} \) is the LJ interaction parameter between polymer and substrate](image)

The second method makes use of the heat capacity. The heat capacity is plotted as a function of temperature. Different approaches have been used in the literature to determine the glass transition temperature from the calorimetric data. In our method, the temperature at the onset of heat capacity rise is defined as the fictive temperature. The
temperature at the peak is called the peak temperature. The glass transition region is defined as the region between these two temperatures. At the peak temperature, the glass transition starts (upon cooling), at the fictive temperature, the glass transition is completed.

![Temperature dependence of $C_p$ for ungrafted film. $e_{ps}=1$](image)

*Figure 2: Temperature dependence of $C_p$ for ungrafted film. $e_{ps}=1$*

In the third method, the local translational mobility of the monomers in the film has been studied. The mean squared displacement (MSD) for different temperatures is calculated. MSD data have been used to obtain the glass transition temperature from molecular dynamics simulations using mode-coupling theory (MCT). The MSD data are employed to calculate relaxation times as a function of temperature. A critical temperature is the temperature at which the relaxation time diverges. The intermediate diffusion constant is defined as:

$$< R^2(t) > = (D_\alpha t)^\alpha$$

where $D_\alpha$ is the diffusion constant, and $\alpha$ is the relaxation time. $< R^2(t) >$ is the mean squared displacement of the beads.

According to MCT, the characteristic time of the translational $\alpha$-relaxation in the sub-diffusive regime, $\tau_r=D_\alpha^{-1}$, algebraically diverges at the critical temperature as:

$$\tau_{tr} = \frac{\tau_0}{(T - T_c)^\gamma}$$

These methods have been used for four different films; grafted films with weak and strong interactions with the substrate, and ungrafted films with weak and strong
interactions with the substrate. The interaction between polymer and substrate is defined by the parameter $\varepsilon_{ps}$. Weak interaction is defined by $\varepsilon_{ps}=0.1$, strong interaction by $\varepsilon_{ps}=1$.

In table 1, the results for the different methods are summarized.

Table 1: Glass transition temperatures obtained using different methods. The first column is obtained using the film thickness, the second using the temperature at which the specific heat starts to rise, the third as the temperature where the specific heat peaks, and the fourth is obtained using the diffusion method. These results are obtained by [1].

<table>
<thead>
<tr>
<th></th>
<th>$T_g^{oper}$</th>
<th>$T_f$</th>
<th>$T_g^{peak}$</th>
<th>$T_c$</th>
</tr>
</thead>
<tbody>
<tr>
<td>ungrafted, $\varepsilon_{ps} = 1$</td>
<td>0.51</td>
<td>0.32</td>
<td>0.5</td>
<td>0.36</td>
</tr>
<tr>
<td>grafted, $\varepsilon_{ps} = 1$</td>
<td>0.54</td>
<td>0.33</td>
<td>0.55</td>
<td>0.36</td>
</tr>
<tr>
<td>ungrafted, $\varepsilon_{ps} = 0.1$</td>
<td>0.32</td>
<td>0.45</td>
<td></td>
<td></td>
</tr>
<tr>
<td>grafted, $\varepsilon_{ps} = 0.1$</td>
<td>0.49</td>
<td>0.33</td>
<td>0.49</td>
<td></td>
</tr>
</tbody>
</table>

In our study, a fourth method to find the glass transition is examined. A thin grafted polymer film is studied. The radial distribution function in the film is calculated. The maximum of the first and second peak is of interest, because they can tell in which state the polymer film is. The maximum depends on temperature. In the glassy state, the maximum stays almost constant. In the liquid state, the maximum of the peak increases linearly with $1/T$.

The maximum of the radial distribution function is related to the local density of the film, and hence to the film thickness.
2. Molecular model and algorithm of simulation

The films, studied in this report, are supported by a substrate on one side. The other side of the film is free (figure 3).

![Figure 3: Thin polymer film, supported by a substrate on one side, the other side being free. (a) non-grafted, (b) grafted](image)

There are two types of film. One film is grafted the other is non-grafted. A polymer is grafted when several beads of the monomer are connected to the substrate via an extra potential. In the grafted film, 25% of the polymers in the film are connected to the substrate. These connections are on average through 4.8 monomers of the polymer.

In the plane of the film, which has a fixed size of 19x16σ, there are periodic boundary conditions in x and y direction.

The particles in the substrate are fixed to their positions in an FCC lattice with a lattice parameter of 0.8σ. The distance between substrate particles is different from the distance between monomers (∼1σ) along a chain to prevent the polymers from positioning along the lattice of the substrate.

The entanglement length $N_e$ of the 40 polymer chains is estimated to be 45 beads [2]. This means that the total number of monomers in a chain is about $2N_e$. In the film, the interaction between the different monomers is due to the Lennard-Jones potential [3],

$$U_{ij}^{LJ} = 4\varepsilon^* \left[ \left( \frac{\sigma}{r_{ij}} \right)^{12} - 2 \left( \frac{\sigma}{r_{ij}} \right)^6 + 0.008742 \right]$$

$$U_{ij}^{LJ} = 0 \quad r_{ij} > 2.2\sigma.$$

An extra potential, the FENE (Finitely Extensible Nonlinear Elastic) potential, is introduced, to represent the bonds in the model. This potential describes the interaction between nearest neighboring particles along a polymer’s chain and the interaction to graft a polymer to the substrate. The FENE potential acts between the bonded beads, as well as the LJ potential.

$$U_{ij}^{FENE} = -\frac{1}{2} kR_0^2 \ln[1 - \left( \frac{r_{ij}}{R_0} \right)^2] \quad r_{ij} < R_0 = 1.5\sigma$$

$$U_{ij}^{FENE} = \infty \quad r_{ij} > R_0$$
The Lennard-Jones potential is cut off at \( r_{ij} = 2.2\sigma \), to neglect the influences of particles further away.

The distance in a chain between particles \( i \) and \( j \) at which \( U_{ij}^{LJ} \) is at a minimum, the equilibrium distance, is approximately \( r_{ij} = 0.96\sigma \). There are 100 monomers in one chain; the end-to-end distance of one polymer is approximately \( 10\sigma \).

It is not a purpose of this study to map the results onto those for real polymer films. The only thing that can be researched with our model and is of interest in this report is the general behavior of the polymer films. All further parameters will be presented in reduced units in which \( \sigma = \varepsilon = m = k_B = 1 \).

In the simulation, the film is divided in layers. This can be seen in the density profile (figure 4).

![Figure 4: Bead density as a function of distance (z) from the substrate for an ungrafted film at a reduced temperature \( T = 0.45 \).](image)

In our case, the film is divided in 14 layers. The first layer is \( 1.45\sigma \) thick; the other 13 are \( 0.9\sigma \) (figure 5). \( \sigma \) is normally chosen in the LJ-potential to be between 0.4-1nm. In the computer program used, the z-coordinate is between \( 35.65\sigma \) and \( 48.8\sigma \). At the substrate, the z-coordinate at the first row of particles is \( 48.8\sigma \). At the free surface, the z-coordinate is around \( 35.65\sigma \).
Figure 5: Layering of the thin film. $48.8\sigma$ is at the substrate, $35.65\sigma$ is at the free surface.
3. Calculating glass transition with radial distribution function

3.1 Theory

To calculate the glass transition temperature, we make use of the radial distribution function [7]. A first step in defining the radial distribution function is the configurational distribution $P(r^N)$. This is the probability distribution for observing a system at configuration space point $r^N$. Integrating this radial distribution function gives us:

$$P(2/N)(r_1,r_2) = \int \int \int \int \int P(r^N) \, dr_3 \, dr_4 \ldots dr_N$$

This is the joint probability distribution for finding particle 1 at position $r_1$ and particle 2 at $r_2$. The joint distribution function for finding a particle (any one) at position $r_1$, and any other particle (in the N particle system) at $r_2$ is $\rho^{(2/N)}(r_1,r_2)$. It is defined as:

$$\rho^{(2/N)}(r_1,r_2) = N(N-1)P(2/N)(r_1,r_2)$$

The radial distribution function is defined in function of this joint distribution function.

$$g(r_1,r_2) = \rho^{(2/N)}(r_1,r_2)/\rho^2$$

where $\rho$ is the density of the material. For an isotropic fluid, this function depends only upon $|r_1-r_2|=r$. Therefore, we can write

$$g(r_1,r_2)=g(r)=G(r)$$

3.2 Simulation

All the simulations are performed on an ungrafted film, unless stated otherwise. $\varepsilon_{ps}=1$

The radial distribution function ($G(r)$) tells us in which way the monomers in the thin film are locally ordered, and at which distance they are from each other.

In the program, a monomer is chosen out of the middle layer of the thin film, lying between 39$\sigma$ and 47$\sigma$ (see figure 6). The distance to all the other monomers is calculated. A histogram is made from all the different distances. This procedure is repeated for every monomer in the film. The radial distribution function is calculated for particles lying between 39$\sigma$ and 47$\sigma$. The radial distribution function of the particles outside this range is not used. This would give an incorrect idea because the particles at the surface of the film are not completely surrounded by other particles. The information obtained is all placed in the same histogram. At the end, the histogram is divided by the total number of monomers used, and by the volume.

This method is used on data for temperatures $T$ between 0.1 and 1.6. The temperature is expressed in units of $\varepsilon/k_B$. The radial distribution function is also calculated two-dimensionally. The term two-dimensionally is used to indicate that for the calculation of the radial distribution function only the particles that are at a distance smaller than 1 by $z$-direction are included. This is just a thin layer of the film, surrounding the tagged
particle. In contrast, in the three-dimensionally case, we consider the whole film, and not only a thin layer. In the following part, we shall use a term “2D simulation” for calculation in a thin layer, and 3D simulation for calculation in the whole film.

Figure 6: 3D pair correlation function for a temperature 0.55T. The relative number of monomers at a certain distance versus the distance is plotted.

In figure 6, we see that the peaks in the pair correlation function are splitted. The split is due to the correlation of the monomer with its two nearest neighbors. Each monomer in the chain is connected to two other monomers, except for the ends of the chains. The FENE potential represents the bonds between those beads. Due to this potential, the split peak appears. When we leave out this interaction with its two neighboring beads, the split peak in the figure disappears (figure 7). This split peak has been observed before [8]. At large distance, the radial distribution function becomes 1.
Figure 7: 3D pair correlation function for temperature 0.55T. The split peak disappears if the interaction between the monomer and its nearest neighbors is left out of the calculation.

Once the pair correlation function is obtained for each temperature, the maximum value of the first and second peak is determined. The inverse of the maximum of these peaks is plotted versus temperature. Above the glass transition, the temperature is linear related to $1/G(r)_{\text{max}}$. If the glass transition temperature is reached, the relation between $1/G(r)_{\text{max}}$ and the temperature stays linear, but the slope of the curve changes. The crossover of those two curves defines the glass transition temperature.
Figure 8: Inverse maximum of the first peak of the radial distribution function versus temperature. 3D simulation.

Figure 9: Inverse maximum of the second peak of the radial distribution function versus temperature. 3D simulation.
In figures 8&9, the inverse maximums of the first and second peak of the radial distribution functions are plotted versus temperature. The glass transition temperature in both plots lays at $T \approx 0.5$, which is in agreement with earlier results [4,5].

The same simulation is performed two-dimensionally. For every particle, only the monomers, with a difference in $z$-coordinate no larger 1, are included in the calculation. The number of monomers averaged over, is less then in the 3D simulation. Therefore, there is more noise in 2D.

![Figure 10: Radial distribution function for temperature 0.55T. The radial distribution function is calculated two-dimensionally.](image)

The maximum of the first and second peak are calculated. Again, there is a trend visible in both the figures 11&12, but not as clear as in figure 9.
Figure 11: Inverse maximum of the first peak of the radial distribution function versus temperature. 2D simulation.

Figure 12: Inverse maximum of the second peak of the radial distribution function versus temperature. 2D simulation.
3.3 Grafted and non-grafted films

The previous results were obtained for an ungrafted film with strong interaction with the substrate. A next step is to compare different types of thin films. The radial distribution function is calculated for four different types of thin films; grafted and non-grafted films, both with weak and strong interaction with the substrate. The interaction between substrate and polymer is determined by the parameter $\epsilon_{ps}$ in the Lennard-Jones potential. The glass transition temperature for these different films is calculated. In figure 13 and 14, we see a clear difference for grafted and ungrafted thin films. In previous research, this difference has never been seen. At higher temperatures, the non-grafted and grafted curves start to differ. The inverse maximums of the grafted curves are lower than the inverse maximums of the non-grafted curves. Thus the peak of the radial distribution function becomes higher when the thin film is grafted. The radial distribution function is an accurate method to measure the local structure. Non-grafted and grafted films have the same density, but locally, the grafted film is different from the non-grafted film. The height of the first peak in the radial distribution function increases when the film is grafted. In figure 13, the curves are linear fitted. The crossover of these two curves seems to be at $T\approx 0.5-0.55$. The crossover for the grafted film is slightly shifted to a higher temperature, compared with the ungrafted film. Thus the glass transition occurs at higher temperature for grafted than for ungrafted films.

![Figure 13: Inverse maximum of the first peak of the radial distribution function versus temperature. 3D simulation. Circles are non-grafted; squares are grafted. Weak interaction with the substrate.](image-url)
The same is done for the second peak of the radial distribution function.

**Figure 14:** Inverse maximum of the second peak of the radial distribution function versus temperature. 3D simulation. Circles are non-grafted, squares are grafted. Weak interaction with the substrate.

**Figure 15:** Inverse maximum of the first peak of the radial distribution function versus temperature. 3D simulation. Both curves are grafted. Circles have a strong interaction with substrate, squares weaker interaction. The interaction is determined by $\epsilon_{pu}$, the interaction between substrate and polymer. This parameter is adjusted in the Lennard-Jones potential.
As seen in figure 15, the curves for grafted thin films with strong and weaker interactions with the substrate don’t differ a lot. The radial distribution function is more sensitive for grafting than for the interaction with the substrate for already grafted films.

The point of crossover of the two different curves is calculated (table 2&3).

**Table 2: Glass transition temperature for ungrafted and grafted films, weak interaction with substrate.**

<table>
<thead>
<tr>
<th>Weak interaction</th>
<th>Tg 1st peak (figure 13)</th>
<th>Tg 2nd peak (figure 14)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ungrafted</td>
<td>0.57</td>
<td>0.48</td>
</tr>
<tr>
<td>Grafted</td>
<td>0.58</td>
<td>0.59</td>
</tr>
</tbody>
</table>

**Table 3: Glass transition temperature for grafted film, with weak and strong interaction with the substrate.**

<table>
<thead>
<tr>
<th>Grafted film</th>
<th>Tg 1st peak (figure 15)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Weak interaction</td>
<td>0.49</td>
</tr>
<tr>
<td>Strong interaction</td>
<td>0.52</td>
</tr>
</tbody>
</table>

The glass transition temperature for the grafted film is higher than for the ungrafted film. This is the best seen in figure 14, with the second peak. The crossover point is T=0.48 for the ungrafted film and T=0.59 for the grafted film.
3.4 Radial distribution function for immobile beads

In [9], the least mobile beads in the thin film are studied. Only the lower half of the film, the half at the surface, is studied. Joris chose this half of the film, so he could take the first half of the film to have a criterion for immobile beads. The radial distribution function for the immobile beads is calculated, and compared with the radial distribution function of all beads.

The immobile beads are believed to have a higher local density than the other beads. Indeed, in the radial distribution function, the first peak is higher for the immobile beads than the peak averaged over all beads. (figure 16,17,18). The difference in peak heights changes with an increase in temperature from $T=0.3$ till $T=0.35$. Such an increase in temperature corresponds with a thickness variation of the film of 2% [1]. Hence the local density around the immobile beads is approximately 2% higher than in the rest.

![Figure 16: Radial distribution function for immobile beads (dotted line) and all beads (straight line). $T=0.3$](image)
Figure 17: Radial distribution function for immobile beads (dotted line) and all beads (straight line).

$T=0.35$

Figure 18: Radial distribution function for immobile beads (dotted line) and all beads (straight line).

$T=0.45$
4. Density in layers

Figure 19: Bead density as a function of distance (z) from the substrate for an ungrafted film with $\varepsilon_{ps} = 1$ at a reduced temperature $T = 0.55$. $\varepsilon_{ps}$ is the interaction between the polymer and the substrate.

The polymer film is divided in 14 layers (figure 19). The temperature is $T = 0.55$. In the figure 4, the density is shown for $T = 0.45$. The layering is the same as described in section 2. In each layer, the density is calculated. Each layer can be seen as a 2D-film. The radial distribution function in each layer is calculated, without taking into account the monomers lying outside the layer.

The number of beads is high at the substrate, and follows an exponential decay through the film till the free end (figure 20). This indicates that the density is higher near the substrate. This is already seen in figure 19.
In section 3.2, the radial distribution function, averaged over the whole film, is calculated. In this part, the film is divided in 14 layers, and the radial distribution function is calculated for each layer. Each layer is seen as a two-dimensional film. Only the interaction between monomers of the same layer is taken into account. In figures 21 & 22, the radial distribution function for beads in a thin layer of the film is calculated. In figure 21, this layer is between 45.55σ and 46.45σ. In figure 22, the layer is between 41.05σ and 40.15σ.
Figure 21: Radial distribution function of the third layer. Layer thickness is 0.9. The temperature is 0.55T.

Figure 22: Radial distribution of the ninth layer. Layer thickness is 0.9. The temperature is 0.55T.
In each layer of the thin film, the maximum of the first and second peak is obtained. The inverse of these maximums are plotted against the layer number. The higher the density, the higher you expect the peak in the radial distribution function. Thus, according to figures 19&20, the highest peak in the radial distribution function must be at the substrate. It gets lower towards the free surface. These results are shown in figures 23&24.

![Diagram showing inverse maximum of the first peak of the radial distribution function in each layer.]

*Figure 23: Inverse maximum of the first peak of the radial distribution function in each layer.*
Figure 24: The place of the second peak of the pair correlation function in each layer.

As the density decreases, the maximum of the radial distribution function is expected to become smaller. In figure 23, this trend is visible.
5. Intensity function

In the paper “Structural Change Accompanying Volume Change in Amorphous Polystyrene as Studied by Small and Intermediate Angle X-ray Scattering”, by Hynn-Hoon Song and Ryong-Joon Roe, another method to find the glass transition temperature is described [6]. This method starts from the scattering function S(k) (figure 25). S(k) is the Fourier transform of the radial distribution function, in k-space. The scattering function gives a peak at k≈1σ. Above the glass transition temperature, the height of this peak, the so-called amorphous halo, changes with temperature. The higher the temperature gets, the higher the peak. Below the glass transition temperature, the height of the peak hardly changes. So, if we can plot the height of the peak in function of temperature, this might be a good way to look at structure.

The scattering function is calculated for several temperatures for the ungrafted film. The height of the first peak, at k≈1σ, is calculated, and the inverse of this peak is plotted in function of the temperature (figure 26).
According to the theory, the height of the peak should change with a different rate above and below the glass transition temperature. In figure 29, this change isn’t really clear. The height of the peak decreases with increasing temperature.
6. Conclusions

In this paper, the glass transition of a thin polymer film is studied. Three methods are already known to calculate this glass transition. A fourth method is used, which makes use of the radial distribution function. Four different types of thin polymer films are used. There is a grafted film with weak and strong interaction with the substrate and an ungrafted film with weak and strong interaction. Weak interaction means that the LJ interaction parameter $\epsilon_{ps}=0.1$, for strong interaction $\epsilon_{ps}=1$. The glass transition temperature can be calculated from the first peak of the radial distribution function as well as the second peak. For the weak interaction, the first peak gives a glass transition at $T=0.57$ for the ungrafted film and $T=0.58$ for the grafted film. The second peak gives $T=0.48$ for the ungrafted film and $T=0.59$ for the grafted film. If weak and strong interaction is compared for the grafted film, the first peak of the radial distribution function gives $T=0.49$ for weak interaction and $T=0.52$ for strong interaction. The curves for weak and strong interaction don’t differ as much (figure 15) as the curves for grafted and ungrafted films (figure 14). This is an important conclusion! This means that the method of the radial distribution function is more sensitive for grafting than for the interaction with the substrate.

A next step in the study was to investigate if the immobile beads, the beads that move the less in the film, would have another radial distribution function then the other beads. As seen in figure 16, the maximum of the radial distribution function for the immobile beads is higher than for the whole film. This means that the local density around those immobile beads is higher than in the rest of the film. Not only the radial distribution function can be used to determine the glass transition temperature, but also the Fourier transform in k-space, the intensity function. The first peak of this intensity function in k-space, around $k \approx 1\sigma$ is used. When the inverse of this peak is plotted against temperature, a decreasing of the peak is seen with an increasing temperature (figure 26). With the method of the intensity function, the glass transition is not seen very well. With the method of the radial distribution function, we can see the glass transition better.
Acknowledgements

I would like to thank prof. dr A.R.C. Baljon and prof. dr R. Khare for their support and helpful information during my stay at SDSU. Also, I would like to thank dr A. Lyulin for his help and ideas during the internship.

Literature


[9] Billen, J. Percolation properties of immobile particles in simulated thin polymeric films near the glass transition; 2004
Appendix: codes

An overview of the FORTRAN90 codes, used in the report:

* gr3D.f90: Calculates the radial distribution function, averaged over the whole film.

* grlayer2Dflexint.f90: Calculates the radial distribution function in each layer, and integrates the radial distribution function in each layer till the first or second minimum.

* grimmoblayer.f90: Calculates the radial distribution function in a random layer, averaged over all particles in the layer. Calculates the radial distribution function of the immobile particles in the selected layer.

* grimmoblast.f90: Calculates the radial distribution function, averaged over all particles in the film. Calculates the radial distribution function, averaged over all immobile particles in the film.

* sk2D.f90: Calculates the scattering function, two-dimensionally, only taking into account the x- and y-coordinates. Only two dimensions are used in k-space.

* sk3D.f90: Calculates the scattering function, three-dimensionally, taking into account x-, y-, and z-coordinates. Three dimensions are used in k-space.

* max.f90: Calculates the height of the first or second peak of the radial distribution function or scattering function.