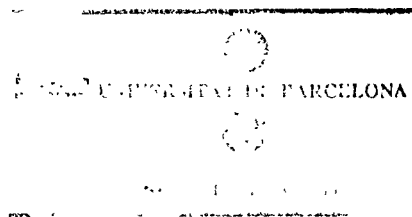


**SIMULACIO MONTE CARLO DE SISTEMES
AMB ACOBLAMENT DE GRAUS DE LLIBERTAT.**



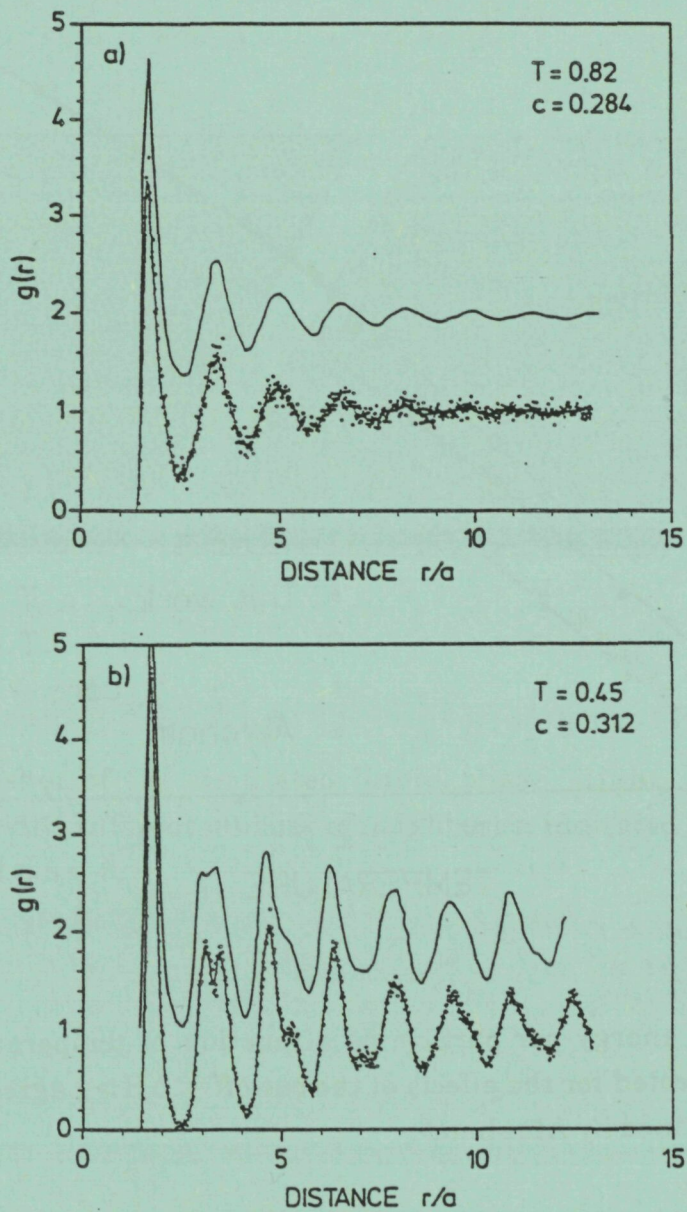


Fig. 4. a) The paircorrelation function $g(r)$ for the liquid phase compared with Abrahams¹⁶ $g(r) + 1$, thin line. b) same for the solid phase.

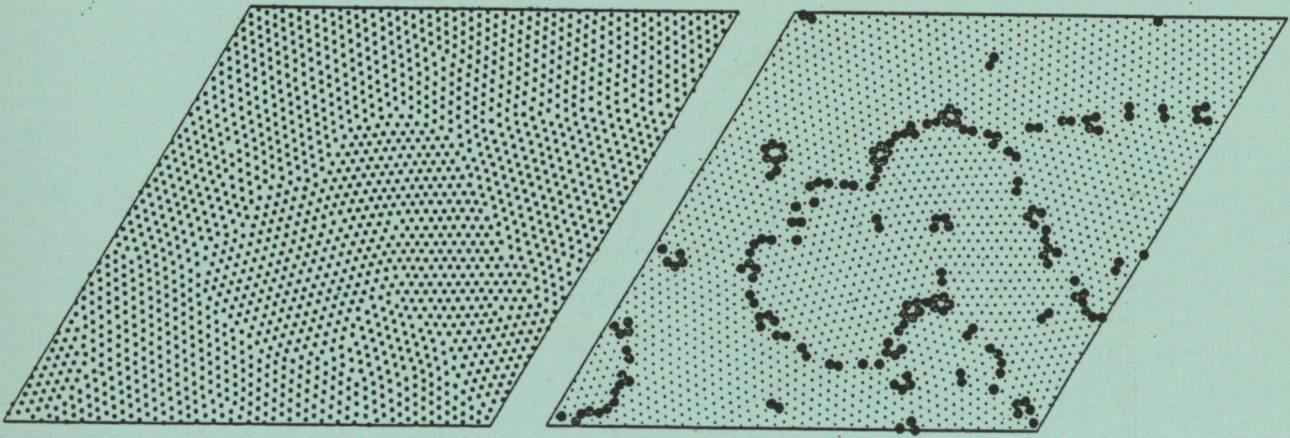


Fig. 5. Left, the solid formed after a quench of a high T liquid after 2000 MCS, $c = 0.3233$, $T = 0.1$. Randomly oriented domains are formed. Right, same with particles with 5 and 7 neighbors indicated by \otimes and \bullet , respectively. Grain boundaries with pairs of 5 - 7 and defects are clearly visible.

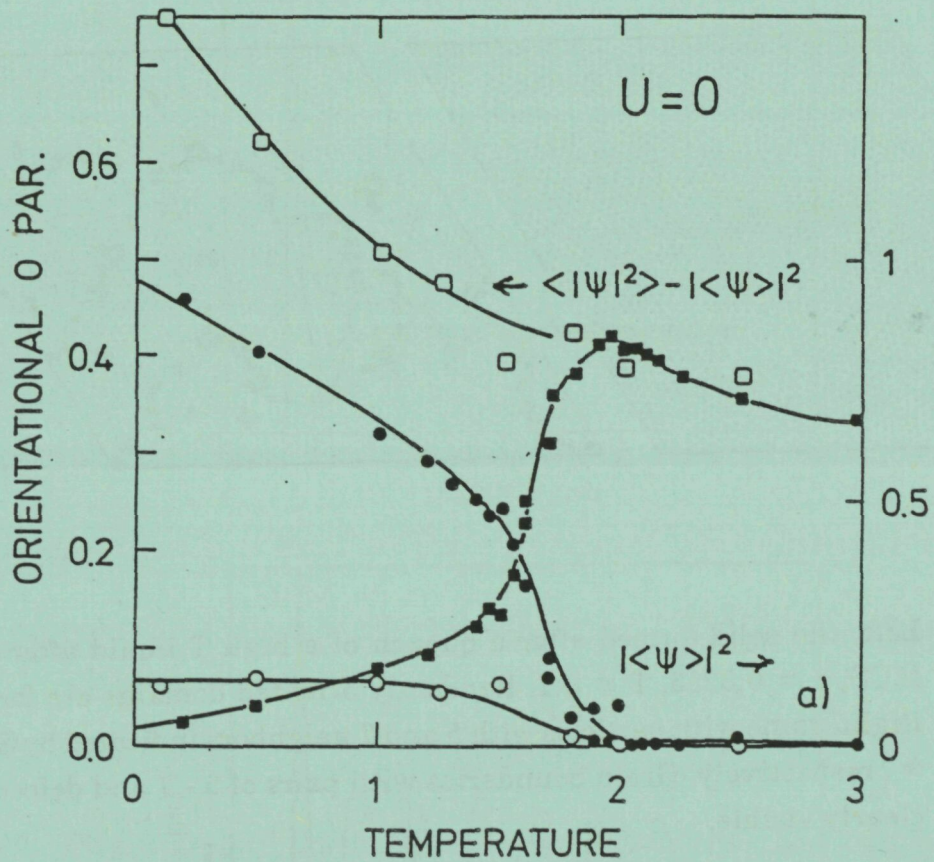


Fig. 6a. The local orientational order parameters $\langle |\psi|^2 \rangle - |\langle \psi \rangle|^2$ (square) and $|\langle \psi \rangle|^2$ (sphere) as a function of T for $U = 0$. The arrows point towards the relevant axes. Clear anomalies occur at $T \sim 2$. Black signatures represent results for heating from a perfect $\sqrt{3} \times \sqrt{3}$ structure and open signatures for cooling from the liquid phase. It shows that crystal growth and melting is irreversible.

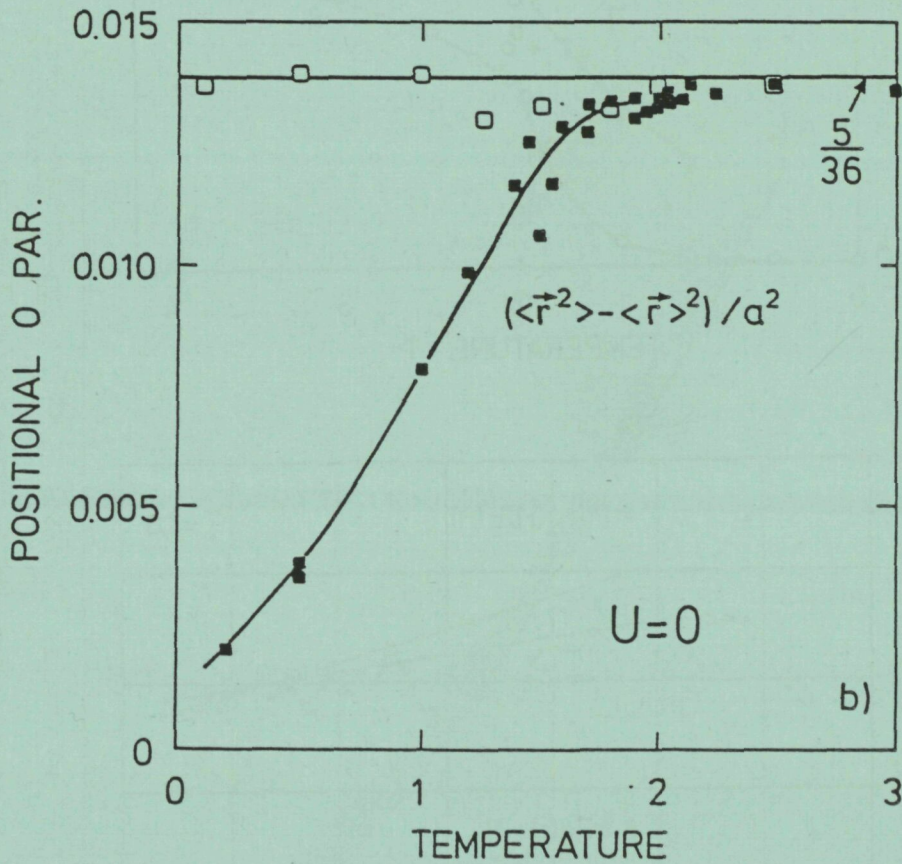


Fig 6b. The positional fluctuation parameter $(\langle r^2 \rangle - \langle r \rangle^2) / a^2$ showing an anomaly at $T \sim 1.55$ close to the low T side of the transition region. The exact high T limit $5/36$ is reproduced, thin line. Notice that upon cooling of the liquid (open symbols), the formed solid has no correlation with the reference lattice.

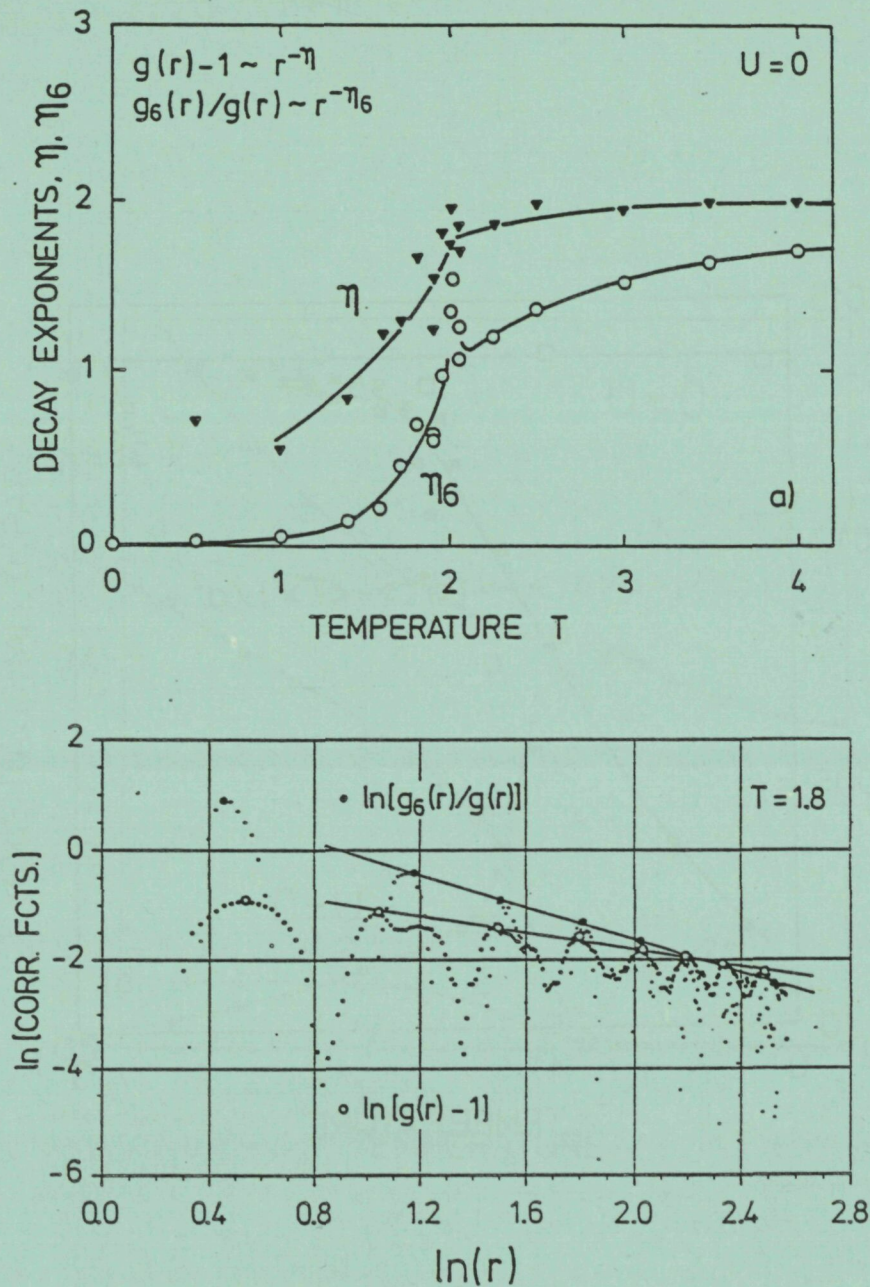


Fig. 7a. Decay exponents η and η_6 for the simple and the orientational pair correlation functions $g(r) - 1$ and $g_6(r)/g(r)$. Clear anomalies occur at $T = 2$ for $U = 0$.

Fig. 7b. Plot of the logarithm of the correlation functions $g_6(r)/g(r)$ and $g(r) - 1$. It demonstrates that the decay is algebraic and not exponential as anticipated by Halperin and Nelson⁴. The symbols \circ and \bullet indicate the maximum of $\ln [g_6(r)/g(r)]$ and $\ln [g(r)-1]$, respectively, and the thin lines are guides to the eye.

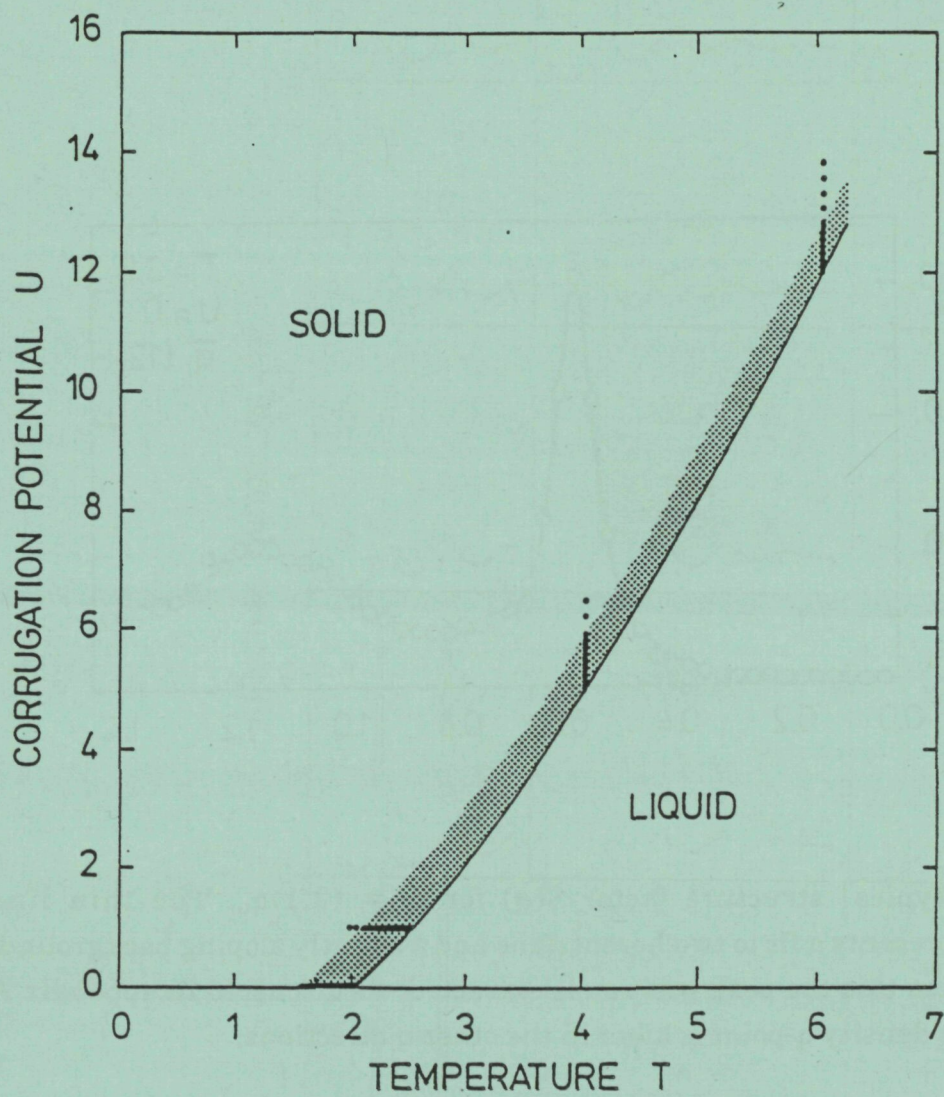


Fig. 8. The phase diagram for coverage $c = 1/3$ as a function of temperature and corrugation potential U . The shaded area indicates the transition region obtained from the indicated scans.

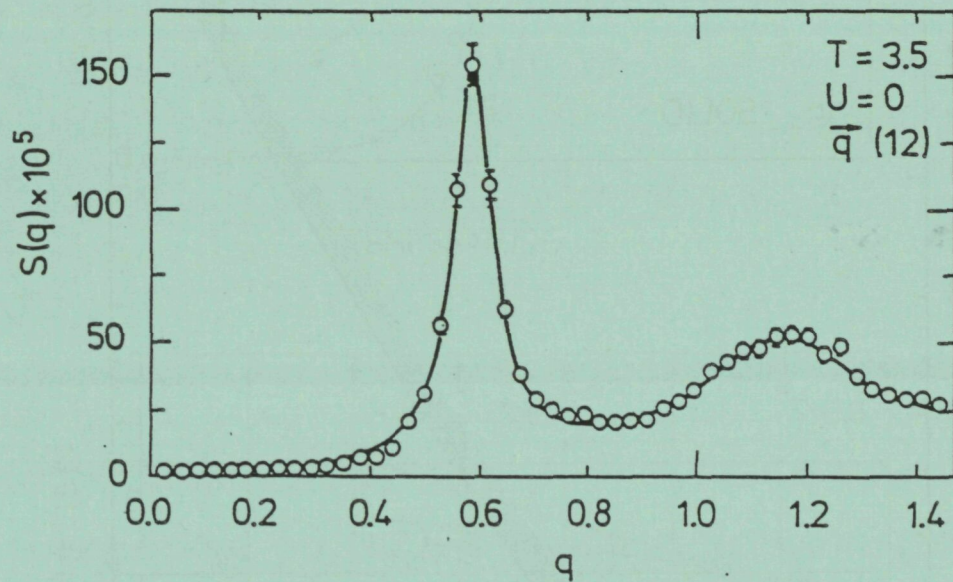


Fig. 9.

A typical structure factor $S(q)$ for $q = (2,1)q_0$. The thin line represents a fit to two Lorentzians and a slightly sloping background. From this the peak position is extracted. As discussed in appendix A the density q -point is higher in the other q directions.

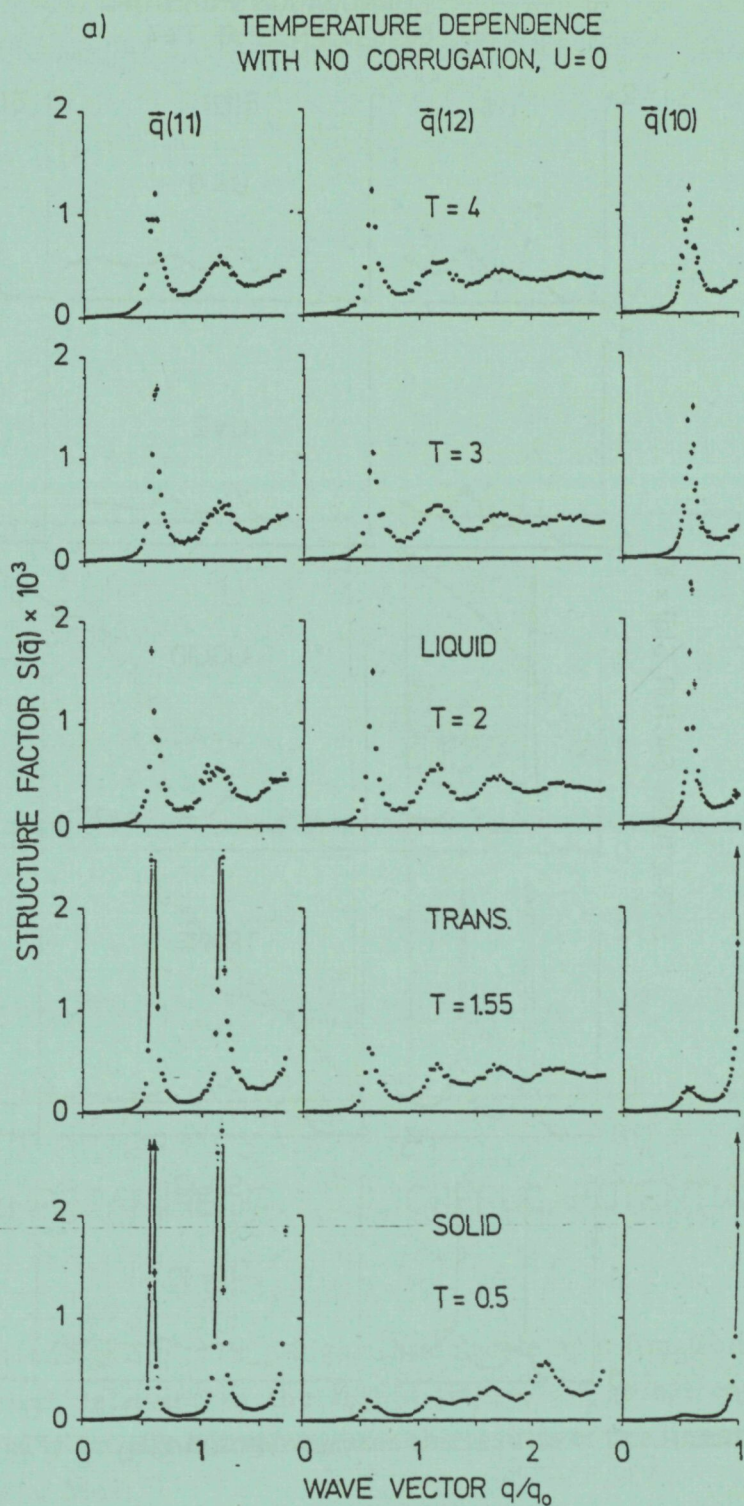


Fig. 10a. Sequence of structure factors for $U = 0$ as a function of temperature T (heating), for three q directions: $q(hk)$ corresponds to $q = (h,k)q_0$. Notice the disappearance of the $\sqrt{3} \times \sqrt{3}$ Bragg peaks at $T = 2$, and the isotropic liquid structure factor at high $T = 4$. Examples from the solid, the transition region and several from the liquid phase are shown.

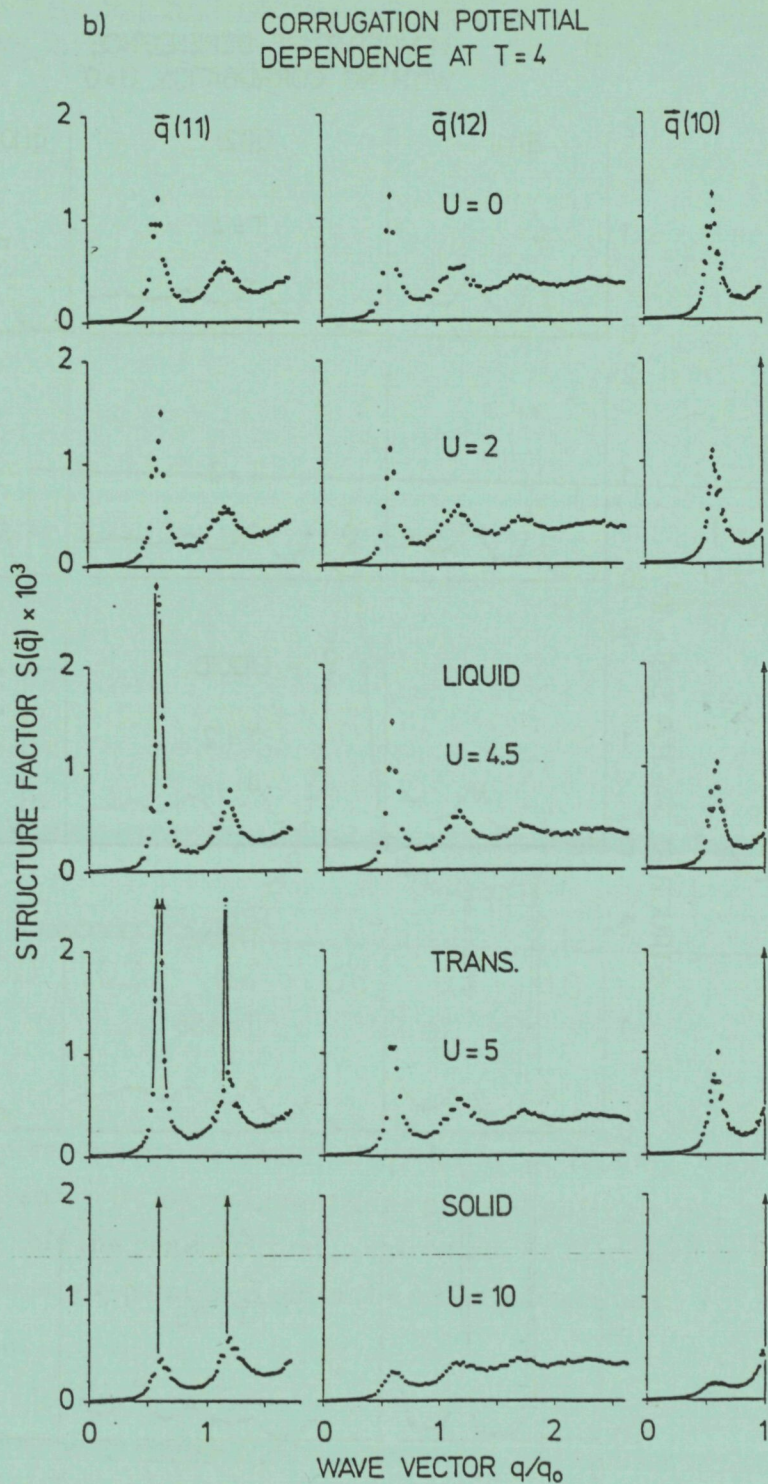


Fig. 10b. Same for constant $T = 4$ and as a function of the corrugation potential U (decreasing). Notice the disappearance of the Bragg peaks along the (11) direction for $U < 4.5$, but the persistence of the (substrate) potential induced (10) Bragg peak. Compare with the phase diagram Fig. 8.

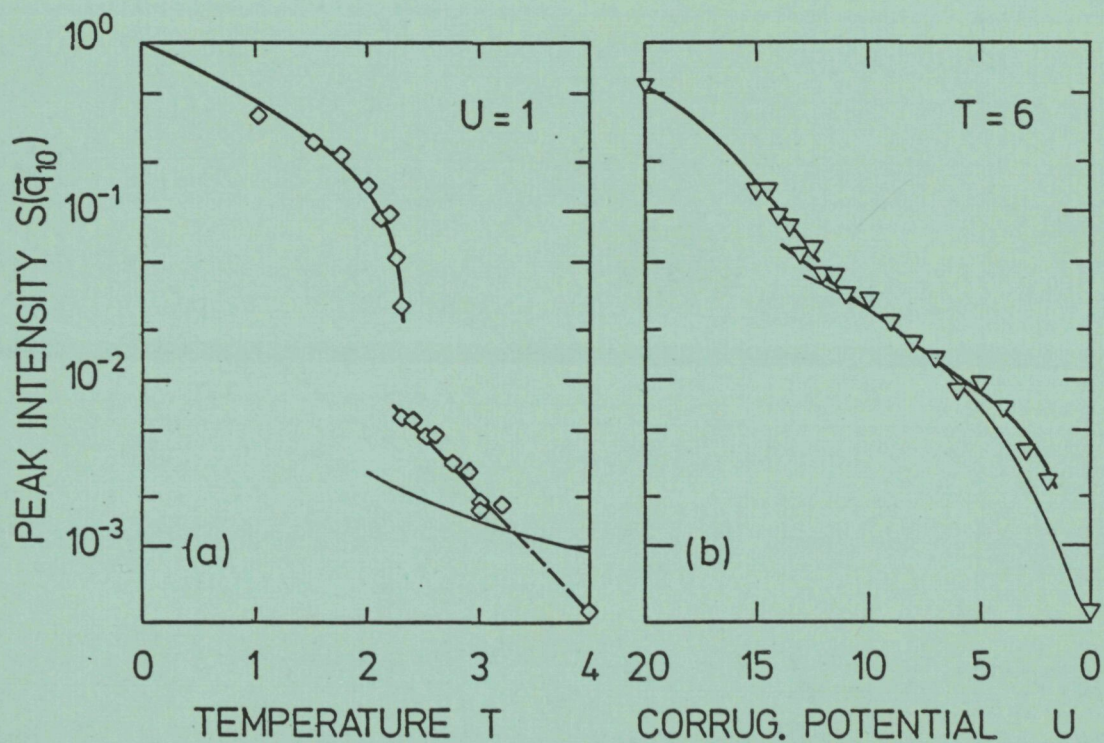


Fig. 11a. Peak intensity $S(q_{10})$ on a logarithmic scale as a function T . Notice the linear behavior in the liquid phase, for small corrugation potential $U = 1$. The line indicates the results of the linear theory by Reiter and Moss²¹.

b. Same as a function of decreasing corrugation potential U for $T = 6$.

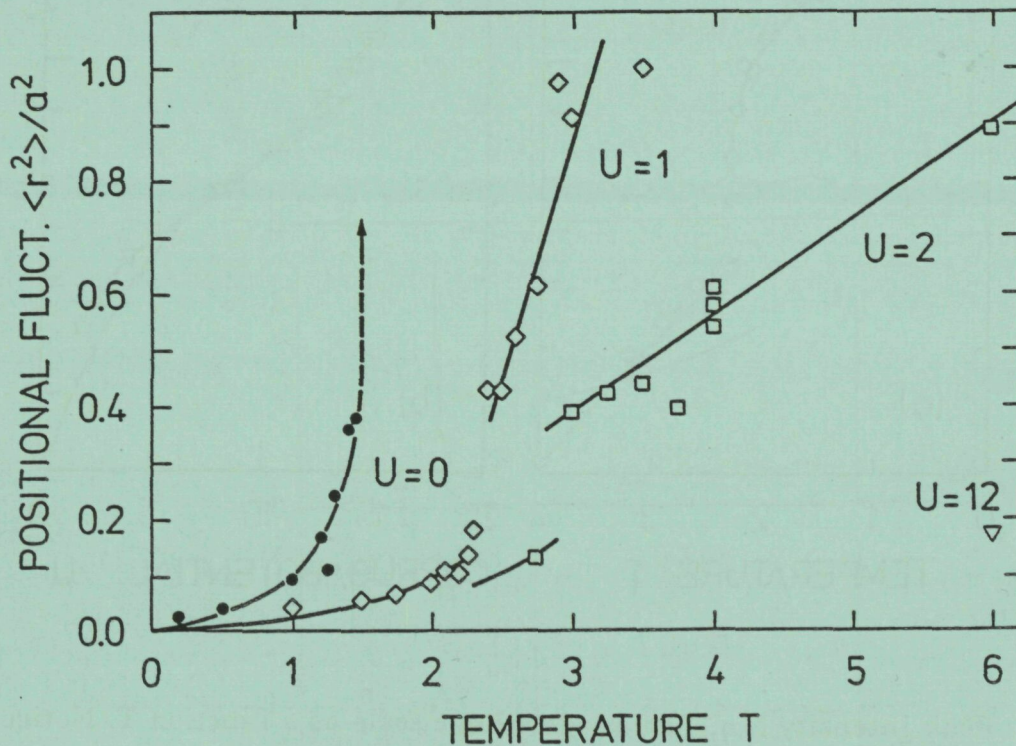


Fig. 12. The calculated positional fluctuation $\langle r^2 \rangle / a^2$ for different value of U . Notice the close to linear increase with temperature for constant U and the expected dramatic increase for $U = 0$. Notice also that for small U $\langle r^2 \rangle / a^2$ is generally much larger near the melting point than for larger U .

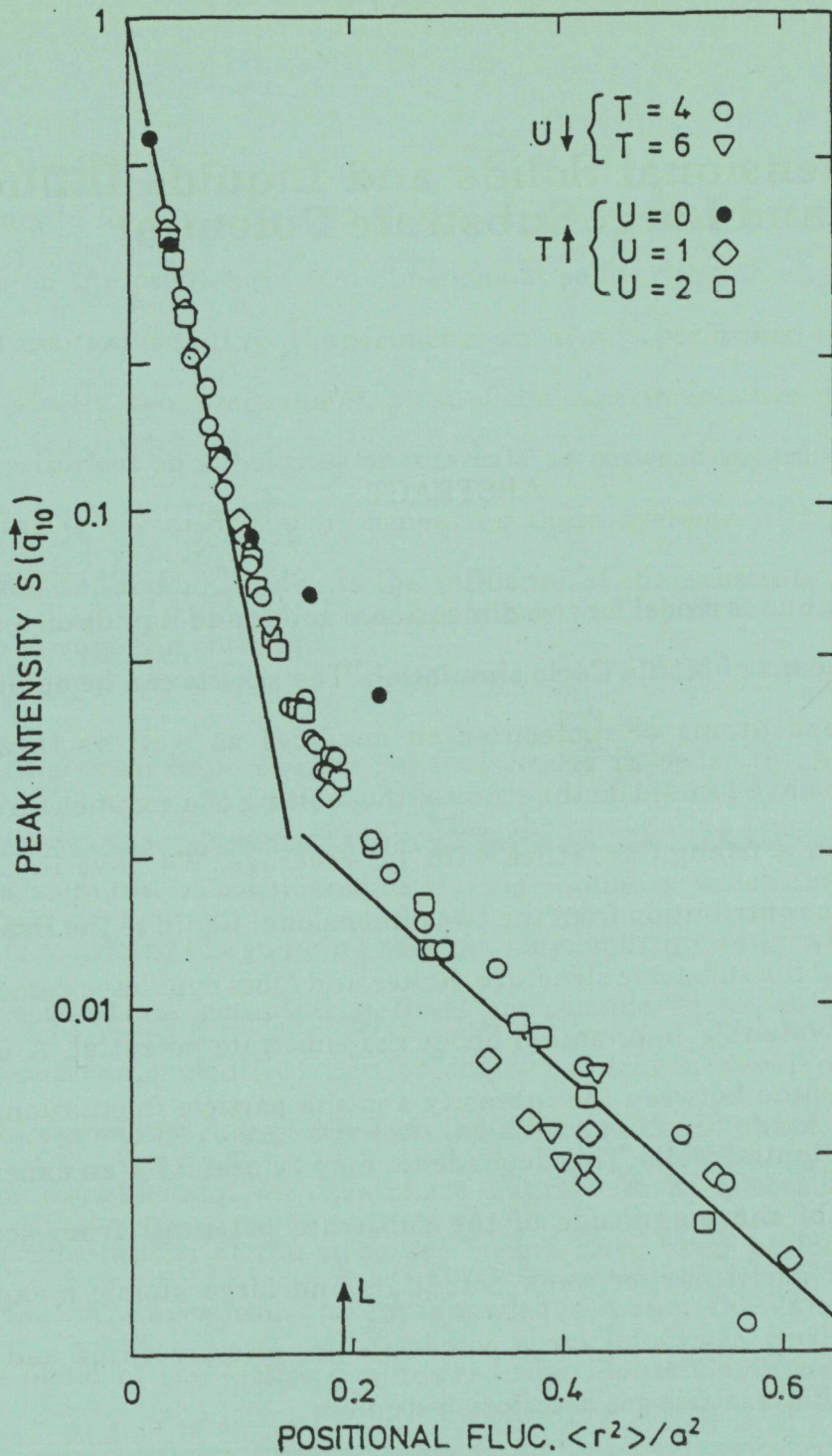


Fig. 13. A Debye-Waller plot showing that the $S(q_{10})$ peak intensity is approximately a universal function of the positional fluctuation parameter $\langle r^2 \rangle / a^2$ for finite corrugation potential $U \neq 0$ and for various T . It is defined in eq. (9). The arrow at L indicates the Lindemann criterion for melting ¹. The transition region in Fig. 8 falls in the range $L \leq \langle r^2 \rangle / a^2 \leq 0.3$.

Two Dimensional Solids and Liquids Influenced by Small and Large Substrate Potential

ABSTRACT

A general, continuous model for two dimensional solids and liquids on a substrate is studied by means of Monte Carlo simulation. The results can be applied to the case of adsorbed atoms or molecules on surfaces as well as intercalated compounds. We have focused on the study of the melting of a commensurate $\sqrt{3} \times \sqrt{3}$ structure on a triangular lattice with $1/3$ coverage. We have in particular investigated the contribution from the two dimensional liquid to the Bragg peaks corresponding to the substrate structure. Reiter and Moss et al have demonstrated that this gives valuable information about the substrate potential. A universal dependence is found between the intensity and the particle fluctuations around the substrate potential wells. This dependence may be useful for an experimental determination of the magnitude of the substrate potential from scattering experiments, in particular for weak potentials and large atomic mean square displacements. New results for large potentials are also presented and possible relations to the Potts lattice gas description studied.

I. Introduction

A main reason for the prolonged discussion, see a recent review¹, and lack of consensus on the problem of two dimensional solids, liquids and specially the melting transition is that real experiments are always performed on systems that are not perfectly two dimensional. Most of the experiments are performed with atoms physisorbed on substrates or intercalated between layers. A main factor contributing to the difficulty in comparing these systems with the ideal two dimensional solids and liquids is the influence of the substrate potential, also called the corrugation potential.

Two limiting cases have usually been discussed in order to characterize the substrate influence. The first assumes that the corrugation potential is large, so that the system can be considered as a lattice liquid in which the motion of the particles is restricted to a jumping between neighbouring wells, while the motion within the substrate potential wells is not considered. In this limit several theories concerning modified Potts Models² have been developed, discussing mainly the symmetry change between the solid and liquid phase. Some of them³ seem to be in agreement with the phase diagram for Kr adsorbed on graphite⁴. Very few calculations of the structure factors have been performed for these models, the only exception, to our knowledge, being the calculation of the structure factor of the lattice gas model using Monte Carlo simulation⁵. The second case studied is based on the assumption that the substrate potential is relatively small and can be considered as perturbing the real continuous liquid. A general perturbation theory of the substrate influence on the structure factor has been developed by Reiter and Moss⁶ and has been proved to be successful in describing experiments on Rb^{7,8} as well as on K⁹ intercalated in Graphite. The theory allows the possibility of extracting the corrugation potential from X-ray scattering data. The principal conclusion of the theory is that the 2d liquid

produces an important contribution to the Bragg peaks of the substrate, and that the diffuse liquid ring structure factor may be reproduced around all the substrate peaks. The linear approximation predicts that the contribution to the Bragg peak intensity of the substrate is proportional to $(V_{\text{HK}}/k_{\text{B}}T)^2$ where V_{HK} are the Fourier coefficients of the substrate potential, T is the thermodynamic temperature and k_{B} is the Boltzmann factor. The intensity of the secondary rings is of higher order. The quantitative comparison between these predictions and experiments is however not easy and therefore molecular dynamics calculations have been used^{8,10} for tests. A main problem with this technique is that only relatively small systems can be studied within reasonable computer time, and finite size effects may influence the results. In a recent paper¹¹ we proposed instead a continuous Monte Carlo method, which allows the possibility of studying systems of 2700 atoms or more, thereby considerably reducing the finite size effects. Here this is further studied by considering very large corrugation potentials, as a step towards unifying the Potts lattice description and the continuous, perturbed liquid description, which is needed in order to understand the influence of the substrate on the two dimensional solids and liquids.

II The Model

The model¹¹ is defined on a 2d triangular reference lattice, with $L \times L$ sites i ($i = 1, \dots, N = L \times L$) and lattice parameter a . Each site in the lattice corresponds to the center of a hexagonal cell representing the substrate with edge length $= a/\sqrt{3}$. On each site of the triangular lattice we define a variable S_i taking the two values 0 or 1 depending on the absence or presence of a particle at the cell i . Further we define \mathbf{r}_i which is a 2d continuous vector that measures the position of the center of the atom inside the cell. We neglect the possibility of perpendicular motion of the particles. The total number of particles on the surface is kept constant so that: