Mechanical and Flow Behavior of Two-Dimensional Foams

Kyozi Kawasaki*, Tohru Okuzono* and Tatsuzo Nagai†

*Department of Physics, Kyushu University 33 Fukuoka, Japan

†Physics Department, Kyushu Kyoritsu University, Kitakyushu 807, Japan

ABSTRACT

A brief overview is given of our recent computer works on mechanical and flow behavior of two-dimensional irregular foams adapting our vertex model used previously for foam coarsening to this problem. Some new simulation data are presented. We include a comment on the results and outline a possible extension of the model.

1. INTRODUCTION

In this article we present a brief overview of our recent investigations on mechanical and rheological behavior of irregular foams deferring the details to other articles which were already published or are being published[1]. This will be followed by new simulation data and a few comments.

Despite the rather long history of research, very little is understood regarding mechanical and flow properties of an assembly of foams[2]. Majority of the previous theoretical investigations of two-dimensional foams is for regular arrays of incompressible identical hexagons where the energy is proportional to the cell boundary length, the so-called Princen-Prud'homme model[2]. Here the cells deform as shown in Fig.1 under externally applied shear strain and the energy and the stress behave as shown in Fig.2. Elastic behavior is periodically interrupted by recombinations of cell boundaries (T-1 processes) such as that shown in Fig.3, which are responsible for both plastic and viscous behaviors as well as for hysteresis. However, the model is a poor approximation to actual irregular foams which do not exhibit such pe-

Fig.1 Deformation of regular hexagonal structure under shear strain.

Fig.2 The energy and stress as functions of strain. The arrows on the solid(dashed) curve indicate directions of change as the strain is increased(decreased).

Fig.3 A recombination of boundaries (T-1 process).

Fig.4 The domain boundary configurations of the original system (left) and that of the vertex model (right).

riodicity. The computer modelling for studying elastic and plastic behavior of irregular foams was pioneered by Weaire and collaborators[3]. Recently we have applied to this sort of problems the simplified model, the so-called vertex model, which was successfully used to study coarsening problems of random cellular systems like grain growth. The model permits us to focus our attention on the motion of intersections of cell boundaries called vertices, which enormously simplify computations. See Fig.4 for an intuitive explanation. Construction of the model and its application to coarsening were already described in great details in [1](a) and (b), and will not be repeated. Thus we go on directly to elastic-plastic properties.

2. MECHANICAL BEHAVIOR[1(c)]

Fig.5 Snapshots of the patterns before (a) and after (b,c) affine deformations are applied, (d) and (e) are the patterns after applying reverse deformations.

In order to stabilize the foam structure which otherwise will coarsen indefinitely and vanish we here suppose that after evolving for a sufficiently

Fig.6(left) The energy versus strain. The arrows indicate directions of change.

Fig.7(right) The normal stress versus strain. The arrows indicate directions of change. The positive and negative histograms are the frequencies of the T-1 processes during the forward and backward deformation processes, respectively.

long time the area of every cell in the system is assumed to stop any further change during the time of measurements in which air diffusion can be neglected. After equilibration we apply a small affine deformation of pure shear type and equilibrate again and monitor the cell pattern obtained and physical quantities such as the energy and the normal stress. We then apply another small affine deformation and repeat the process. Snapshots of the patterns obtained are shown in Fig.5. In this way we find the energy and the normal stress as functions of accumulated applied deformation expressed in terms of the Hencky strain ϵ . That is, the relative shrinking and expansion in the x and y directions are given, respectively, by $e^{-\epsilon}$ and e^{ϵ} . This is shown in Figs.6 and 7. Here the initial elastic response with accumulating stress is occasionally relaxed by the T-1 processes. The system then shows plasticity and hysteresis as shown in Fig.7 together with the frequencies of the T-1 processes. This connection was pointed out first by Ashby and Verrall[4]. It looks as though single sharp jumps occurring periodically in the regular hexagon model are spread over the wider region of deformation in the irregular cell patterns.

Fig.8 Snapshot of the patterns during shear deformation process with a constant rate.

3. FLOW BEHAVIOR[1(d)]

Finally we discuss the flow behavior, in particular, the response of the system to simple shear strain with constant rates. Here we find that the viscous dissipation occurring within parts of the liquid film near Plateau borders plays the dominant roll where the diffusion of gas across the cell boundaries is virtually forbidden. The former dissipation process was studied previously within the lubrication approximation[2] and this result can be used to construct the dissipation function for vertex motions. The vertex equation of motion is readily obtained by balancing the friction force acting on each vertex which is obtained from the dissipation function and the static force derived from the expression for the energy in which the constraints of fixing areas of all the cells are imposed. The effect of an applied strain is taken care

Fig.9(left) Stress as a function of the total strain (proportional to time). Different symbols correspond to different strain rates [1(d)].

Fig.10(right) The average steady state shear stress under a uniform shear flow.

of by replacing the vertex velocity by its relative velocity with respect to the background velocity associated with the applied strain with the constant rate. The boundary condition used is the displaced periodic boundary condition well-known in the non-equilibrium molecular dynamic simulation[5].

We display in Fig.8 snapshots of the patterns at increasing times after application of the shear with a constant rate. The shear stress is shown as a function of the strain (proportional to the time) in Fig.9. We see setting up of steady state regimes at sufficiently long times and hence we can find the average steady state stress τ as a function of the shear rate $\dot{\gamma}$. Preliminary results of such a study were reported in [1(d)]. We have taken more simulation data especially at smaller values of $\dot{\gamma}$. The latest results are shown in Fig.10. This clearly shows the existence of a finite yield stress and is consistent with a finite shear viscosity like a Bingham plastic,

$$\tau = \tau_0 + \eta\dot{\gamma}, \quad (1)$$

where τ_0 and η are positive constants. This differs from what we concluded before on the basis of fewer simulation data[1(d)].

Fig.11 Shear stress vs simple shear strain $\square$ from dynamic and $\bullet$ from static computations.

4. DISCUSSION

Now, it is well known that a simple shear deformation is a combination of a pure shear deformation and a rigid body rotation[6]. Thus our results for the static relation between stress-pure shear strain can be transcribed into the relation between shear stress and simple shear strain $\gamma = \dot{\gamma}t$. In this way we can directly compare static stress-strain relation with the dynamic one. Such a comparison is made in Fig.11. In relating pure and simple shear deformations, we have used the formula[6]

$$\gamma = 2 \cot 2\chi, \quad \chi = \tan^{-1} e^{-\epsilon}. \quad (2)$$

Also we determined the static shear stress corresponding to the simple shear strain γ by rotating the static stress tensor by the angle χ . We have slightly displaced the simulation data points in such a way that the stress vanishes for zero strain. The original data points deviate from this due to the finite system size with non-vanishing statistical fluctuations. The figure shows that the static and dynamic stress-strain relations are very similar at least in the small deformation region. The dynamic result is for a small shear rate chosen ($\dot{\gamma} = 10^{-3}$) and from Fig.9 large discrepancies are expected for larger shear rates. This is simply due to the fact that for larger shear rates the stress accumulates more quickly before relaxing. We also point out that principal axes of the dynamic stress tensor do not generally coincide with those of the static stress tensor because topology changes cannot instantly follow the rotation. In fact our simulation shows that the angle corresponding to χ for the dynamic case approaches a nonvanishing limit as the strain increases indefinitely.

5. EXTENSION OF THE MODEL

Up to now the shear deformation and hence the average local velocity $u(r)$ were assumed to be externally imposed. However, in actual experiments only the velocity at the system boundary can be imposed and the average local velocity within the system is the unknown that has to be determined by some supplementary conditions. We here outline a way to deal with this problem. In the approximation of the Stokes flow without inertia effects, such supplementary conditions are provided by the condition of mechanical equilibrium on every coarse-graining volume in the system. Here a coarse-graining volume is so chosen that a large number of cells are contained in it but its size is much smaller than the distance in which macroscopic variation of physical quantities such as $u(r)$ can take place. Here the term "macroscopic" is used as an antonym of "microscopic" meaning the level of individual cells. This condition is expressed in terms of the microscopic expression for the local stress tensor $\hat{\tau}(r)$

$$\nabla \cdot \langle \hat{\tau}(r) \rangle = 0, \quad (3)$$

where the angular bracket denotes statistical averaging. If time variation is very slow, we can neglect dissipative contributions to $\hat{\tau}(r)$ that contain fluid viscosity. Then $\hat{\tau}(r)$ consists of two parts, namely, a contribution from cell boundaries $\hat{\tau}_b(r)$ and that containing the local pressure inside individual cells $p(r)$:

$$\hat{\tau}(r) = \hat{\tau}_b(r) - p(r)\mathbf{1}, \quad (4)$$

where $\mathbf{1}$ is the two-dimensional unit tensor. For the vertex model $\hat{\tau}_b$ takes the form

$$\hat{\tau}_b(r) = 2\sigma \sum_{\langle ij \rangle} |r_{ij}| \hat{r}_{ij} \hat{r}_{ij} \delta(r - \frac{r_i + r_j}{2}), \quad (5)$$

with $\hat{r}_{ij} \equiv r_{ij}/|r_{ij}|$ and $r_{ij} \equiv r_i - r_j$ where r_i is the position vector of the vertex i , σ is the surface tension of one side of the cell boundary and the summation is over the pairs of vertices i, j directly connected by a cell boundary. We may eliminate the unknown $p(r)$ by assuming that the total pressure p_0 is spatially constant since any inhomogeneity will be quickly dissipated by sound waves. Hence

$$T_r \hat{\tau}(r) = -2p_0, \quad (6)$$

and thus

$$p(r) = p_0 + \frac{1}{2} T_r \hat{\tau}_b(r), \quad (7)$$

where T_r is trace of a tensor. This is substituted into (4) to find that $\hat{\tau}(r)$ is simply the traceless part $\hat{\tau}_b^{TL}$ of $\hat{\tau}_b$ apart from a constant. Thus the condition (3) simply becomes

$$\nabla \cdot \langle \hat{\tau}_b^{TL}(r) \rangle = 0. \quad (8)$$

If self-averaging property is assumed for our problem the average in (8) may be replaced by the average over a coarse-graining volume. A way to implement this is to make use of a set of independent functions $\psi_s(\mathbf{r})$ whose number equals that of the coarse-graining volumes which fill up the system volume and to replace (8) by

$$\int d\mathbf{r} \psi_s(\mathbf{r}) \nabla \cdot \hat{\tau}_b^{TL}(\mathbf{r}) = 0. \quad (9)$$

The condition (9) can then be incorporated into the vertex equation of motion by the vector Lagrange multipliers μ_s . This equation which generalizes that of [1(d)] is now written as

$$\begin{aligned} & \frac{6}{5} \frac{\partial}{\partial v_i} R(\{v_j - u(\mathbf{r}_j)\}, \{v_j\}) + \frac{\partial}{\partial r_i} H(\{\mathbf{r}_j\}) \\ & = - \sum \frac{\partial}{\partial r_i} \left\{ \sum_{\alpha} \lambda_{\alpha} A_{\alpha} + \sum_s \mu_s \cdot \int \psi_s(\mathbf{r}) \nabla \hat{\tau}_b^{TL}(\mathbf{r}) d\mathbf{r} \right\}, \quad (10) \end{aligned}$$

where R and H are, respectively, the dissipation function and the free-energy of the vertex model with v_i the velocity of the vertex i , and A_{α} is the area of the cell α and λ_{α} is the Lagrange multiplier that keeps A_{α} constant. The extra factor $\frac{6}{5}$ in front of the first term on the lhs of (10) reflects the fact that R is not a quadratic function of $v_j - u(\mathbf{r}_j)$ but contains that variable raised to the $\frac{5}{3}$ power. A natural choice of $\psi_s(\mathbf{r})$ is to take it to be unity in the coarse-graining volume s and zero outside. On the other hand, computationally it may be easier to choose other functions like plane wave functions. The Lagrange multipliers λ_{α} and μ_s can be determined from the conditions that the time derivatives of A_{α} and that of the lhs of (9) vanish where $\psi_s(\mathbf{r})$ does not depend on time. If $u(\mathbf{r})$ is expanded in the functions $\psi_s(\mathbf{r})$ its expansion coefficients can be determined from (9).

ACKNOWLEDGMENT

K.Kawasaki would like to thank the Yamada Science Foundation for the travel support that enabled him to attend this conference. This work was partially supported by the Scientific Reserch Fund of the Ministry of Education, Science and Culture of Japan.

REFERENCES

- [1] (a) K. Kawasaki, T. Nagai and K. Nakashima, *Phil. Mag.* **B60** (1984), 399
(b) K. Kawasaki, T. Nagai and S. Ohta, in *Simulation and Theory of Evolving Microstructures*, eds. M. P. Anderson and A. D. Rollett (T. M. S. Publication, Warredale, 1990)
(c) K. Kawasaki, T. Nagai and T. Okuzono, in *Microscopic Aspects of Nonlinearity in Condensed Matter*, ed. V. Tognetti (Plenum Press, New York, 1991)
(d) K. Kawasaki, T. Okuzono, T. Kawakatsu and T. Nagai, in *Proceedings of International Workshop on Physics of Pattern Formation*, ed. S. Kai (World Scientific, Singapore, 1992)
- [2] A. M. Kraynik, *Ann. Rev. Fluid. Mech.* **20** (1988), 325
- [3] D. Weaire and J. P. Kermode, *Phil. Mag.* **B50** (1984), 379
D. Weaire and T. L. Fu, *J. Rheol.* **32** (1988), 271
J. P. Kermode and D. Weaire, *Computer Phys. Comm.* **60** (1990), 75
- [4] M. F. Ashby and R. A. Verrall, *Acta Metal* **21** (1973), 149
- [5] M. P. Allen and D. J. Tildesley, *Computer Simulation of Liquids* (Clarendon Press, Oxford, 1987)
- [6] A. S. Lodge, *Elastic Liquids* (Academic Press, London and New York, 1964) Chapter 2.