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Effect of shear energy upon bubble nucleation under shear flow field

MING-CHENG GUO
Institute of Plastics Machinery and Engineering, Beijing University of Chemical Technology, Beijing 100029, People's Republic of China

YU-CHENG PENG*, YE-BIN CAI, WEN-GUAN ZHOU
College of Industrial Equipment and Control Engineering, South China University of Technology, Guangzhou 510641, People's Republic of China
E-mail: pskcgong@sohu.com

Conventional nucleation theory assumes that bubble nucleation is a thermodynamic process and the main driving force is the degree of supersaturation. Although much research has been devoted to the foaming theory, most of the work was aimed at the batch processing. For bubble nucleation in a static polymer melt, the explanation using the conventional classical nucleation theory is still satisfactory, but for the nucleation process in flow fields, using the conventional theory alone is inadequate.

Recently, several models have been proposed to explain the shear effects upon bubble nucleation in shear flow fields. During the heterogeneous nucleation, a modified cavity model was built to show the effect of shear force on bubble detachment from the cavity [1]. And for the homogeneous nucleation, according to the deformation of a single gas bubble under simple shear flow, Chen proposed a cell stretch model to show the enhancement of shear stress upon bubble nucleation [2], and the capillary number was selected to interpret its contribution to the Gibbs free energy that must be overcome for bubble nucleation. But in this model, only a few parameters in the flow fields were included and the shear stress was believed as the critical factor that affected bubble nucleation. But in light of the study of Han and Han [3], melt flow was conceived as another important driving force for bubble nucleation. Therefore, more comprehensive analysis is required in order to fully interpret the shear effect upon bubble nucleation.

As referred by Lee [1] and Chen [2], the investigation of shear effect upon bubble nucleation from the point of view of shear energy is more reasonable since the key of shear nucleation was the transformation of mechanical shear energy into the surface free energy. In this paper, the contribution of shear energy to the Gibbs free energy was analyzed and was incorporated in the classical nucleation theory to interpret the enhancement of shear effect upon bubble nucleation.

For bubble nucleation in a static polymer melt, the bubble surface free energy can only come from the potential energy and the heat energy of the system, while under shear flow fields, more types of energy exist, such as the kinetic energy, which also can be used for bubble nucleation. And this transformation from kinetic energy to the surface free energy can be achieved though the shear energy. Therefore, due to the existence of shear energy in shear flow field, the Gibbs free energy will be reduced relatively.

In another paper [4], we have calculated the shear energy w in unit time and on unit area along the thickness of a slit channel die. During bubble nucleation, since the critical bubble nucleus is very small and of the order of magnitude of hundreds of angstrom [5], the capillary number will be small and therefore the nucleus deformation can be neglected. Suppose the radius of the spherical nucleus is r^*, then for bubble nucleation under shear flow field, the Gibbs free energy can be shown as

$$\Delta G^{**} = \Delta G^* - kw^{3/2} \cdot \frac{4}{3}\pi r^{*3}$$

where ΔG^* is the original Gibbs free energy required for bubble nucleation without shear flow field, k is the efficiency of transformation from shear energy to the surface free energy. And the bubble nucleation rate N in the classical nucleation theory [5–7] can be modified as

$$N = Cf\ \exp(-\Delta G^*/KT)\exp\left(kw^{3/2}\frac{4}{3}\pi r^{*3}/KT\right)$$

where C, f, K, T are the content of nucleation sites, the frequency factor of impinging upon the bubble nucleus for the outer gas molecules, the Boltzmann constant, and the absolute temperature, respectively. It shows that the bubble nucleation rate will increase owing to the existence of shear energy.

To testify the correctness of the above analysis and to prove its applicability in practice, the shear nucleation experiments were made using a slit channel die; details of the experimental setup have been shown in a previous paper [4]. The SEM (scanning electron microscope) cell structures of the extruded sheets at different screw rotation speeds are shown in Fig. 1.

By dividing the images into 10 uniform sections along the thickness direction, the difference of cell

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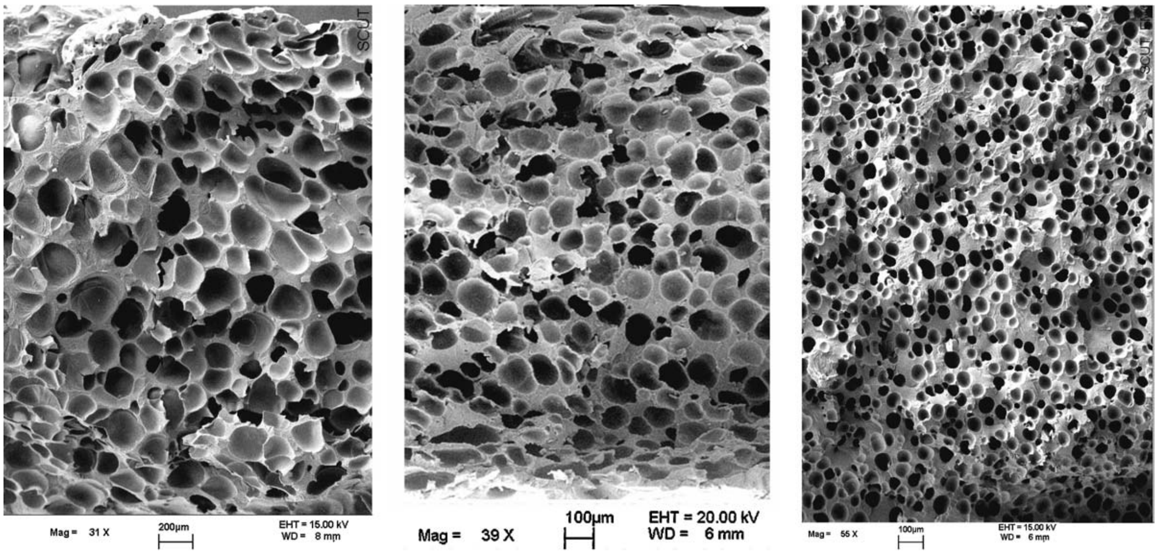
*Author to whom all correspondence should be addressed.



a) b) c)

Figure 1 Cell structures of the fracture surfaces perpendicular to the flow direction for different screw rotation speeds: (a) 5 rpm, (b) 10 rpm and (c) 20 rpm.

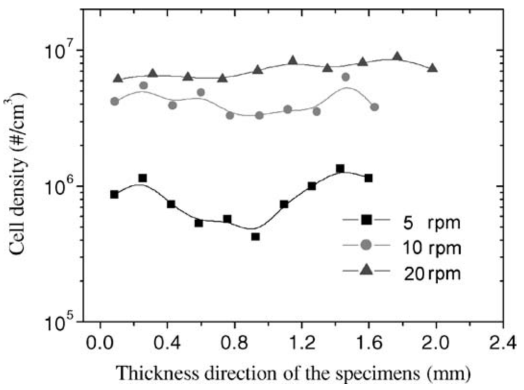


Figure 2 Variation of cell densities along the thickness of the specimens for different screw rotation speeds.

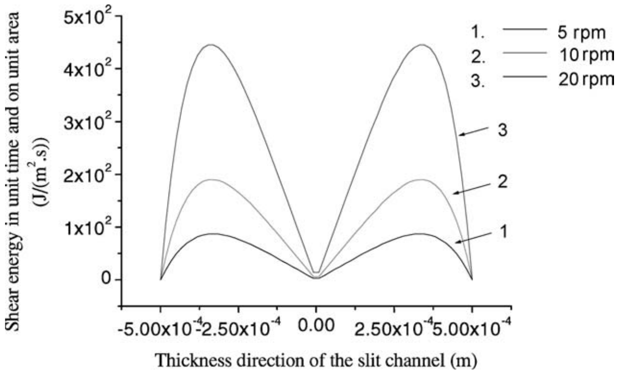


Figure 3 Shear energy in unit time and on unit area along the thickness of the slit channel for different screw rotation speeds.

densities for different sections can be illustrated, as shown in Fig. 2. It can be found that the distribution of cell densities for the low screw rotation speed is in accordance with the result in the literature [2], that is, the cell densities near the wall are higher than those at the center. With the increase of the screw rotation speeds, the difference diminishes gradually, and the cell densities for different sections increase universally.

For a slit channel die, the distribution of shear energy along its thickness also can be calculated according to the experimental conditions, as shown in Fig. 3. By comparing Fig. 2 with Fig. 3, we can find that these curves are very similar at low screw rotation speeds; the higher the shear energy the higher the cell densities. Therefore, the bubble nucleation process under shear flow field can be well described by the shear energy effect. But with increase of the screw rotation speeds, the difference of the curves for shear energy and cell density also increases, and for the condition of 20 rpm, the two curves are altogether different. As seen from the variation of shear energy under different screw speeds, we can find that the shear energy at the die wall and the centerline is always zero, while the maximum shear energy changes. Therefore, with the increase of the screw rotation speed, the unevenness of the shear energy along the thickness of the slit channel increases accordingly, which will enhance the energy transfer from the high energy section to the low energy section. As a result, the shear energy will be more evenly distributed and in turn the difference of cell densities at different sections decreases.

In conclusion, the effect of shear energy upon the Gibbs free energy and the bubble nucleation rate is analyzed under shear flow field. Since the kinetic energy also can be used for bubble nucleation through shear energy, therefore, the Gibbs free energy will be reduced relatively, and the bubble nucleation rate will increase accordingly. The shear nucleation experiments were made using a slit channel die, and the distributions of cell densities along the thickness of the extruded sheets were compared with the distributions of shear energy along the thickness of the slit channel. The results showed that the curves of shear energy and cell densities coincided well with each other under low screw rotation speeds, indicating that the bubble nucleation process under the shear flow field could be well described by the shear energy effect. With the increase of screw rotation speeds, the distribution of cell density gradually deviated from the shear energy curve, and the cell densities along the thickness of the specimen became more uniform, which could be explained by the increase of the unevenness of shear energy under higher screw rotation speed and the energy transfer along the thickness direction.

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