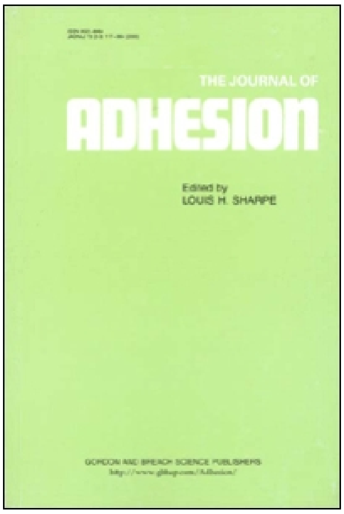

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Interfacial Contact and Bonding in Autohesion I-Contact Theory

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Interfacial Contact and Bonding in Autohesion

I-Contact Theory

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ABSTRACT

A two stage theory, consisting of contact establishment as the first, and bond formation as the second stage, is proposed for autohesion. A viscoelastic contact theory is worked out based on the shape of the surfaces, the contact pressure, and the temperature. Contact of two spheres of polystyrene and a practical surface consisting of cylinders and flats are analyzed mathematically by extending the classical Hertz elastic contact problem by employing elastic-viscoelastic analogy developed by Alfrey and Gurnee. Karam's fourteen element generalized Voigt model is used for computations.

INTRODUCTION

AUTOHESION or self-adhesion is bonding of two adjacent surfaces of the same material compared to adhesion which concerns bonding of different materials. The surfaces should be able to flow and coalesce after contact to result in autohesion. This suggests two stages for this mechanism. In the first stage, which is a primary requirement for autohesion, a contact is established. The shape of the surfaces, the nature of the material comprising them, and the contact pressure, or the force field are the controlling factors. In the second stage, which forms the basis for the self-diffusion theory of autohesion by Voyutskii [1], coalescence takes place by vanishing of the boundary between the two surface layers.

According to Voyutskii theory, complete coalescence occurs instantaneously after contact for low molecular liquids due to high mobility of their molecules. However, for high molecular liquids, such as high polymers, the macromolecules are not so mobile, and it takes some time to achieve complete coalescence. Coalescence in such materials is accomplished by diffusion movement of the macromolecules (macrobrownian) or their segments (microbrownian).

The self-diffusion theory, therefore, describes primarily the processes taking place in the second stage of autohesion, mentioned above. This stage does not exist in case of low molecular liquids due to immediate coalescence after contact. Thus, the theory does not hold for such liquids. In case of high molecular liquids, the two stages are discrete with the coalescence stage lagging behind the contact stage. Once again, this theory is inadequate because it does not account for the first stage which is a primary requirement for autohesion.

THEORETICAL DEVELOPMENTS

The initial contact, when two surfaces are brought together in a certain force field, is at the flat portions of the surface, which increases as their deformation takes place. The increase will depend on the nature of the material.

Usually autohesion takes place when the material is capable of flowing. To analyze the flow of contacting surfaces, use is made of the deformation theory of elastic, viscous, and viscoelastic materials developed by Alfrey and Gurnee [2]. The theory is easily applied to analyze the flow of rough surfaces made by a combination of holes, spheres, and cylinders or their segments as shown in Figure 1. (See following page.)

Elastic-Viscous-Viscoelastic Deformation Theory:

For an isotropic medium, the deviatoric stress and strain tensors are related through the shear modulus G by

$$s_{ij} = 2Ge_{ij} \tag{1}$$

where s_{ij} is the stress and e_{ij} is the strain.

For an ideal Newtonian liquid, shear stress is proportional to shear strain rate through a constant of proportionality called the viscosity η. The equation (1) for such liquids may be written as:

$$s_{ij} = 2\eta\dot{e}_{ij} \tag{2}$$

where $\dot{e}_{ij} = \frac{\partial}{\partial t}(e_{ij})$

By comparing expression (1) with (2) which hold for solids and liquids, respectively, we get the following correspondence operators equation.

$$G \leftrightarrow \eta \frac{\partial}{\partial t}$$

For a simple Voigt model material, shown in Figure 2, the equation corresponding to (2) is

$$s_{ij} = 2Ge_{ij}(t) + 2\eta\dot{e}_{ij}(t) \tag{3}$$

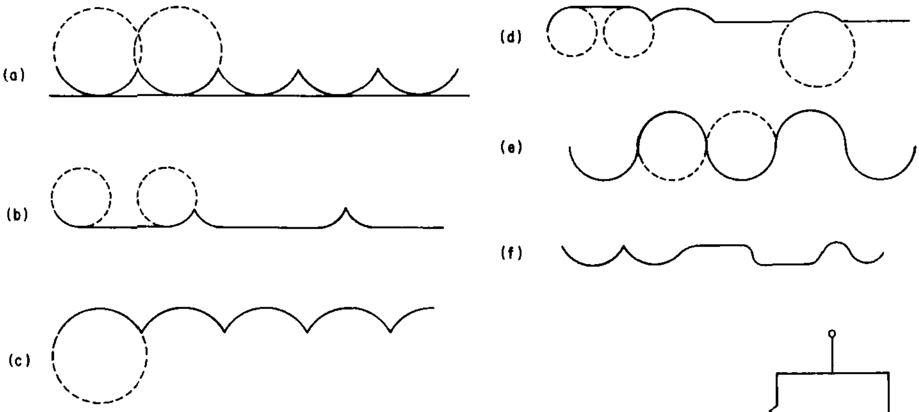

Figure 1. Schematic of Generation of Simple Rough Surfaces by Combination of: (a) Spheres or Cylinders, (b) Spheres or Cylinders and Flats, (c) Spherical or Cylindrical Holes, (d) Holes and Flats, (e) Spheres and Holes, (f) Spheres, Holes and Flats.

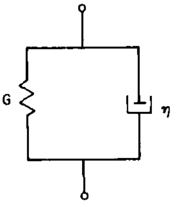

Figure 2. Voigt model.

which gives the following correspondence

$$G \leftrightarrow G + \eta \frac{\partial}{\partial t}$$

If a stress s_o is applied instantaneously the solution of (3) is

$$e_{ij}(t) = \frac{s_o}{2G}\left[1 - e^{-t/\tau}\right]$$

where $\tau = \eta/G$ is the retardation time. This leads to the following correspondence expression

$$\frac{1}{G} \leftrightarrow \frac{1}{G}\left[1 - e^{-t/\tau}\right]$$

For a generalized Voigt material (Fig. 3), the total strain is the sum of the strains in the individual elements. Thus,

$$e_{ij}(t) = \frac{s_o}{2}\left[\frac{1}{G_o} + \sum_{i=1}^{N} J_i\left(1 - e^{-t/\tau_i}\right) + {}^{t}/\eta_o\right] \tag{4}$$

where $J_i = \dfrac{1}{G_i}$ are the compliances and $\tau_i = \dfrac{\eta_i}{G_i}$ are the retardation times. This yields the following correspondence

$$\frac{1}{G} \leftrightarrow \frac{1}{G_o} + \sum_{i=1}^{N} J_i\left(1 - e^{-t/\tau_i}\right) + \frac{t}{\eta_o} \tag{5}$$

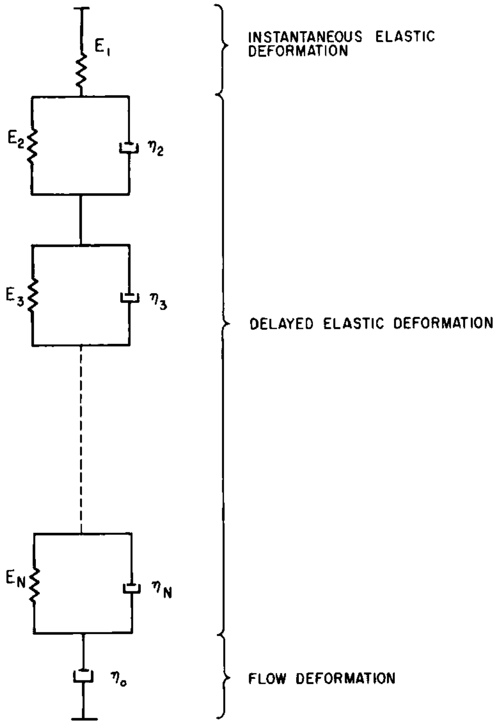

Figure 3. Generalized Voigt model.

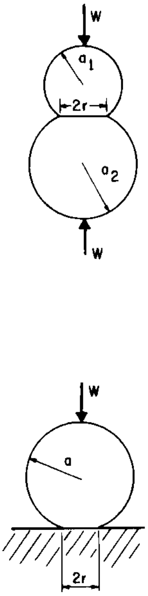

Figure 4. (a) Contact of two spheres, (b) The equivalent problem of contact of a sphere with a flat rigid plate.

Viscoelastic Contact Theory:

An analysis of the problem of viscoelastic spheres and cylinders in contact is given below. This solution may be applied to study deformation of some of the surfaces shown in Figure 1, as mentioned already.

The theory for the classical case of contact of two elastic spheres or cylinders was first worked out by Hertz, in 1886 [3]. For contact of two spheres of radii a_1 and a_2 under a load of W, as shown in Figure 4, the expression determining the radius r of the contact of the surface is

$$k = \frac{3}{16\pi}\frac{W}{r^3}\left(\frac{1-\nu_1}{G_1}+\frac{1-\nu_2}{G_2}\right) \tag{6}$$

where $k = \frac{1}{2}\left(\frac{1}{a_1}+\frac{1}{a_2}\right)$ is the relative curvature

ν_1, ν_2 are the Poisson's ratios
G_1, G_2 are the shear moduli

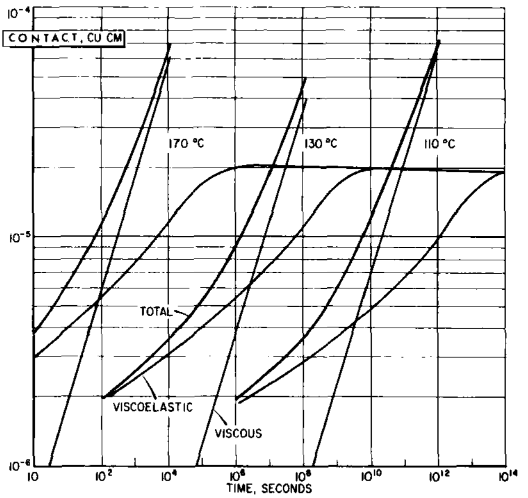

Figure 5. Plot of calculated contact radius cube vs. time for two polystyrene spheres.

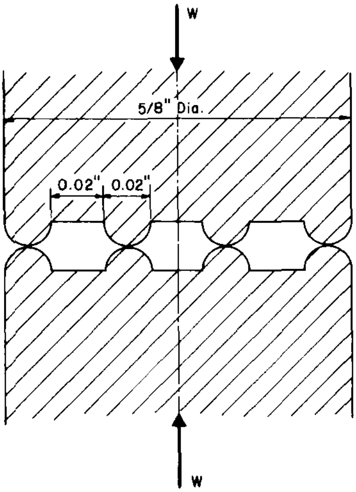

Figure 6. Contact of surfaces made up of cylindrical segments and flats.

The corresponding expression for the half width b of the contact rectangle for cylinders is given by

$$k = \frac{W}{\pi b^2}\left(\frac{1-\nu_1}{G_1} + \frac{1-\nu_2}{G_2}\right) \tag{7}$$

The contact of two spheres or cylinders of the same material is equivalent to that of a single sphere or a cylinder, say of shear modulus G and Poisson's ratio ν, in contact with a flat rigid plate for which the shear modulus and the radius are both infinite. Thus, expressions (6) and (7) become

$$r^3 = \frac{3}{8\pi} Wa\left(\frac{1-\nu}{G}\right) \tag{8}$$

for spheres and

$$b^2 = \frac{Wa}{\pi}\left(\frac{1-\nu}{G}\right) \tag{9}$$

for cylinders, respectively.

For a viscoelastic material which may be represented by a generalized Voigt model (Figure 3), for constant instantaneous loading, G is given by (5).

APPLICATION

The concepts developed so far may now be employed to analyze the contact of surfaces made of polystyrene. A 14 element generalized Voigt model for the general purpose linear, amorphous polystyrene (Styron®

666-PA187) has been proposed by Karam [4]. He has determined the values of the compliance function, the retardation times, and zero shear viscosity from simple creep experiments. The data is listed in the reference cited above, where the constants are given as functions of temperatures. Shift factors for temperatures ranging from 80°C to 170°C are listed too. The instantaneous elastic deformation corresponding to the first element is found to be negligible.

The series form of the above-mentioned creep function, which involves only 14 elements, is very convenient to use in practice rather than a function which has an infinite spectrum of elements. This permits actual computation of the time dependent strains as functions of stress.

Using this model, the expression for the contact radius for two spheres is given by substituting (5) in (8). Thus, we have for $\nu = 0.5$

$$\left(\frac{16\pi}{3Wa}\right) r^3 = \sum_{i=1}^{14} J_i \left(1 - e^{-t/\tau_i}\right) + \frac{t}{\eta_o}$$

Figure 5 is a plot of the radius cube as a function of time for the temperatures 110, 130, and 170°C.

Figure 6 shows contact of surfaces composed of cylinders and flats. Such surfaces occur frequently in practice and their analysis is a useful illustration. The area of contact is plotted as a function of time for temperatures of 100, 120 and 140°C in Figure 7. The curves are terminated when complete contact is attained.

DISCUSSION

The self-diffusion theory of autohesion proposed by Voyutskii is based on the assumption that activation energies of the two processes, viz, autohesion and self-diffusion, have the same order of magnitude. According to this theory a gradual coalescence of the interface takes place by macro- and micro-Brownian motion of molecules or their segments. This theory does not explain the pressure dependence of autohesion since diffusion is not a pressure dependent process.

It may be pointed out that variation of the viscosity with temperature is analogous to that of diffusion and autohesion. The activation energies of the two processes are identical [5]. Also, viscosity controls the rate of deformation of the surface and should explain the effect of pressures. A contact theory is, therefore, proposed wherein elastic, viscous and viscoelastic deformation of surfaces takes place to establish the contact.

It is possible that self-diffusion and contact establishment may be operating instantaneously. Contact theory explains the pressure dependence of

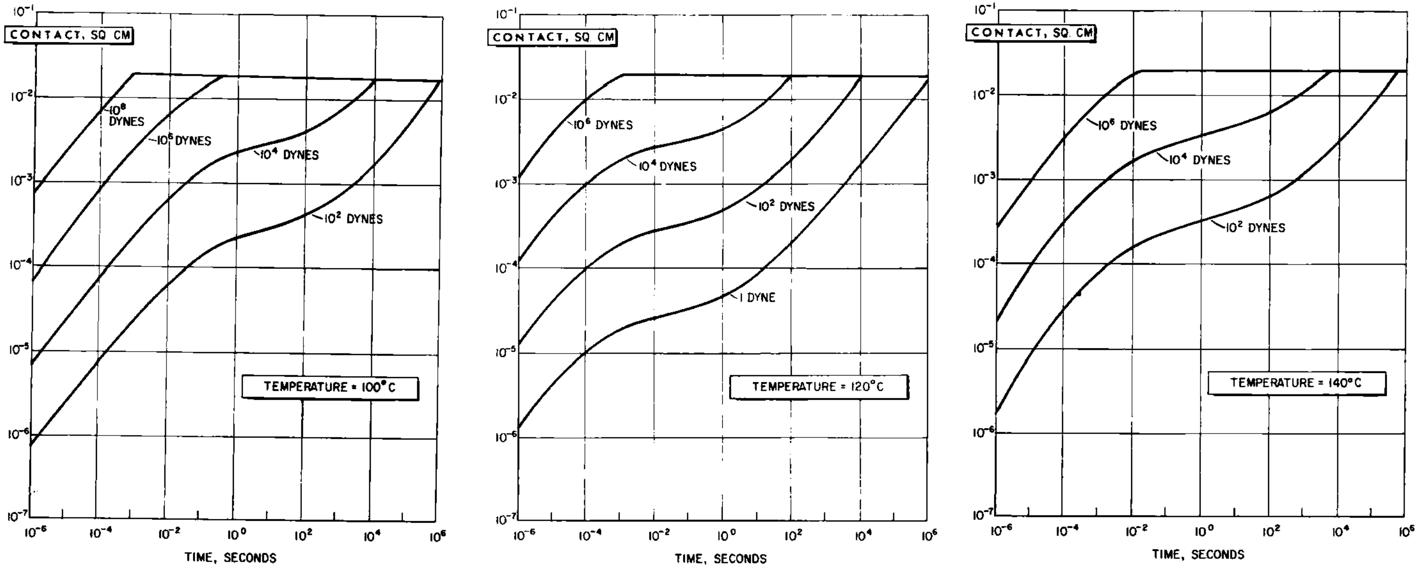

Figure 7. Plots showing calculated rates of contact for various loads—temperatures of: (a) 100°C, (b) 120°C, (c) 140°C.

autohesion in a rather positive and direct manner. It would be reasonable to doubt whether diffusion should be considered at all as a mechanism of autohesion, since its dependence on time, temperature and pressure may all be explained exclusively from the point of view of flow and deformation in establishing contact.

The rate of contact curves are essentially the bonding curves since the latter follow the contact. Bonding and breaking tests have been carried out for the surfaces of Figure 6. These results will be reported in a later paper in this series. They show that the bonding curves are essentially of the same shape as predicted by the contact theory. The change of slope of the curves of Figure 7, due to disappearance of the viscoelastic component, occurs at approximately the same time.

Hertz elastic contact theory has been extended to the viscoelastic case by the use of elastic-viscoelastic analogy. This theory is limited to small deformations only, but in the past, researchers have been able to fit the data for large deformations to a semi-empirical form of the Hertz equation. This subject has been reviewed recently by Chapoy and Aklonis [6]. We have employed the fourteen element generalized Voigt model for polystyrene which yields a good fit even for high deformations. This eliminates the necessity of fitting the data to an empirical equation as needed in case of a single element model.

NOMENCLATURE

s_{ij}, s_o = shear stress
e_{ij} = shear strain
G, G_o, G_1, G_2, G_i = shear modulus
η, η_o, η_i = viscosity
J_o, J_i = compliance
a, a_1, a_2, = sphere, cylinder radius
ν, ν_1, ν_2 = Poisson's ratio
r = radius of contact
k = relative curvature
t = time
τ_i = retardation time
W = load
b = half width of contact rectangle
π = 3.1416
$\frac{\partial}{\partial t}$ = partial derivative w.r.t. time
$\sum_{i=1}^{N}$ = summation for $i = 1$ to N

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