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### Interfacial Contact and Bonding in Autohesion: III-Parallel Plate Attraction

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# Interfacial Contact and Bonding in Autohesion:

## III-Parallel Plate Attraction

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### ABSTRACT

Interfacial bonding force at the interface of polystyrene is computed by considering interaction of repeat units constituting molecules on the two sides. The interaction force between the repeat units is obtained from the 6-12 Lennard-Jones potential curves determined previously. The maximum value of the bonding force is of the same order of magnitude as the yield stress. Results indicate that regions in the immediate vicinity of flat regions where separation is within about 20A contribute to the overall strength of the bond.

### INTRODUCTION

**I**NTERFACIAL bonding force at the contact surface of polystyrene is primarily due to London dispersion type of van der Waals forces. These forces exist between the repeat units that constitute molecules on the two sides of the interface. The 6-12 Lennard-Jones potential curve, the gradient of which determines the above forces, has been obtained in the previous paper [1].

At the flat contact regions, surfaces approach each other up to a minimum equilibrium separation. Strength of the interfacial bond here is the yield stress of the polymer. However, the overall bond strength is lower due to existence of regions which are not flattened out. As deformation proceeds with time, so does the interfacial bonding, and finally, as the surfaces are flattened out completely, the interfacial bonding approaches the yield stress.

The bonding force may be obtained from the attraction between parallel plates, as calculated by Hamaker [2]. This does not apply strictly in the regions where surfaces are not flat but the separation is still of molecular order. However, from a knowledge of the shape, the force may still be obtained by assuming the parallel plate formula to hold over a differential area and integrating over the whole area. To be precise, though, the force of attraction should be calculated with an accounting for the shape of surfaces.

Hamaker calculated the force of attraction between two semi-infinite parallel plates from van der Waal's forces. These forces fall off inversely as the sixth power of distance. The force per unit area of the plates is calculated to be

$$f = \frac{A}{6\pi d^3}$$

where  $d$  is the separation and  $A$  is the Hamaker constant. The value of  $A$  for polystyrene is of the order of  $32 \times 10^{-13}$  erg. [3]. The expression does not hold for values of  $A \rightarrow 0$ , since the force becomes infinite. However, at smaller distances, the short range repulsive force due to interference of electrostatic fields comes into play.

By using a 6-12 Lennard-Jones potential Good [4] has extended Hamaker's calculations to bring in the repulsive component. The material is thought of as a continuum; whereas, in fact the attraction is a result of interaction between discrete molecular repeat units. Thus, these calculations should be performed by considering the interaction of discrete individual units. This involves summation over an infinite number of units. However, beyond a certain distance, the contribution of interactions is negligible, which makes possible a direct computation.

In the case of polystyrene, the contribution of units beyond about twenty atomic distances is negligible. Given below are the calculations.

### INTERFACIAL BONDING

One needs to know the relative positions of the interacting units in order to compute their contribution. Although the repeat units of a molecule do not occupy any symmetrical arrangement, it is assumed, for simplicity of mathematics, that they have a simple cubic packing as shown in Figure 1. The lattice parameter for this packing may be taken as the equilibrium separation of these units in their crystal lattice [1]. Thus

$$r_0 = 7.30 \text{ \AA}$$

The force between two units at a distance  $r$  may be derived from the 6-12 Lennard-Jones potential. Thus, the force  $F(r)$  is [1]

$$F(r) = 6B \left( \frac{1}{r^7} - \frac{2p}{r^{13}} \right) \quad (1)$$

where

$$p = \frac{1}{2} (r_0^6)$$

The value of  $B$  determined in the previous paper from a comparison of the cohesive energy and the lattice energy is

$$B = 1.428 \text{ dyne A}^7$$

Figure 1 also shows schematically how the individual units interact to yield a net normal component of the attractive force. The tangential components all vanish because of symmetry. The force  $f$  between any two units at a distance  $r$  is

$$f(r) = F(r) \cos \theta(r) \quad (2)$$

where

$$\cos \theta = \frac{x}{r}$$

The value of  $x$  and  $r$  in terms of the lattice distance are

$$x = (l + d) r_0 \quad (3)$$

$$r = [(l + d)^2 + m^2 + n^2]^{1/2} r_0$$

where  $l, m, n$  are integers, and  $d$  is the separation between the plates. The total force  $f'$  on unit  $A$  in the left plate due to interaction with all the units in the other plate is obtained from (2) to be

$$f' = \sum_r f(r) \quad (4)$$

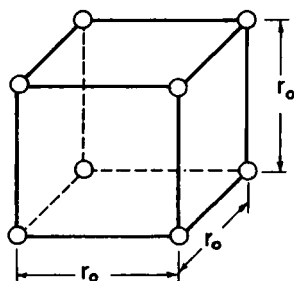
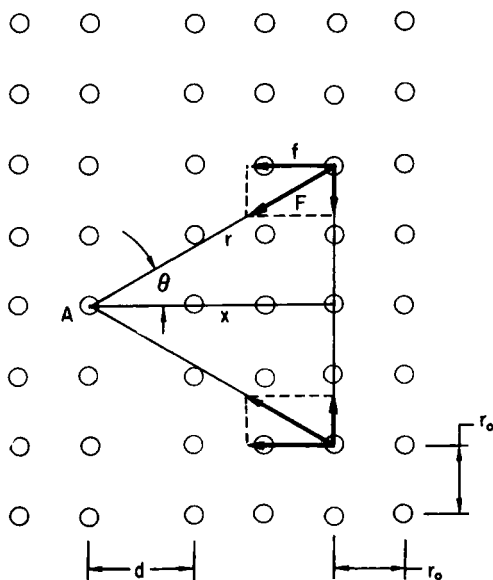


Figure 1. Simple cubic arrangement of the molecular repeat units showing interaction to yield a net normal attractive component. The tangential components vanish from symmetry.

Substituting (1) and (3) in (4), we get

$$f' = \frac{3B}{r_0 p} [(\Sigma)_4 - (\Sigma)_7] \quad (5)$$

where

$$(\Sigma)_s = \sum_{l=1}^{\infty} \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} \frac{l+d}{[(l+d)^2 + m^2 + n^2]^{-s}}$$

for  $s = 4$  or  $7$

This force may then be summed over all the units on the left of the plate directly behind the facing unit to yield the total force over an area of cross-section  $a$  of

$$a = r_0^2$$

The value of  $d$  for these units is replaced by

$$D = d - lr_0$$

The force  $f''$  is therefore

$$f'' = \sum_{l=0}^{-\infty} f'$$

and the stress  $\sigma$  is

$$\sigma = f''/a$$

If  $B$  is in dyne  $A^7$  and distances are in Angstroms, the units of  $\sigma$  are dyne/ $A^2$  which may be converted into dyne/cm<sup>2</sup> by multiplying by a factor of  $10^{16}$ . This may then be converted into units of p.s.i. by the conversion factor

$$1 \text{ p.s.i.} \approx 6.9 \times 10^4 \text{ dyne/cm}^2.$$

## RESULTS AND DISCUSSION

Calculations are performed by use of a digital computer where the infinite series are terminated at a point beyond which the contribution of units to force is negligible. The results are shown in Figure 2 where the force per unit area is plotted against the separation between faces.

The curve is similar to the stress strain plot of polystyrene. The maximum value that corresponds to the maximum bonding force is about 7500 psi. This value is comparable to the experimentally determined value of about 6000 psi for general purpose polystyrene. This agreement suggests that the main contribution to the interfacial bonding would be from London dispersion type of van der Waal's forces.

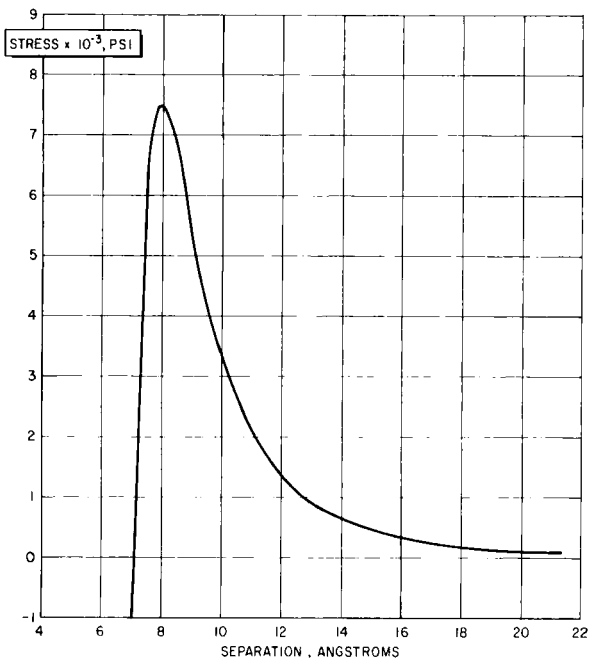


Figure 2. Plot of the calculated force per unit area between parallel plates vs. separation.

Variation of this force with separation indicates that the force falls off gradually with distance. Beyond separation of about 20A, the force is negligible. In the case of rough bodies in contact, however, contribution of faces apart up to separations of 20A should be considered. The contact regions therefore include besides the flat areas the neighboring regions where separation is within the above limit. These regions are usually quite large because of the fact that the flat regions taper off gradually.

The force vs. separation curve may be applied to the problem analyzed in the first paper (5) viz. contact of surfaces consisting of cylinders and flats. The results are shown in Figure 3 where plots of relative strength vs. time are shown for various loads for temperatures of 100°, 120°, and 140°C. Experimental verification of these by performing bonding and breaking tests has been carried out. The procedure and results will be discussed in a future paper. The bond strength curves have the same general shape as predicted. The transition from viscoelastic to viscous deformation occurs at the same time as predicted by using tensile creep data of polystyrene.

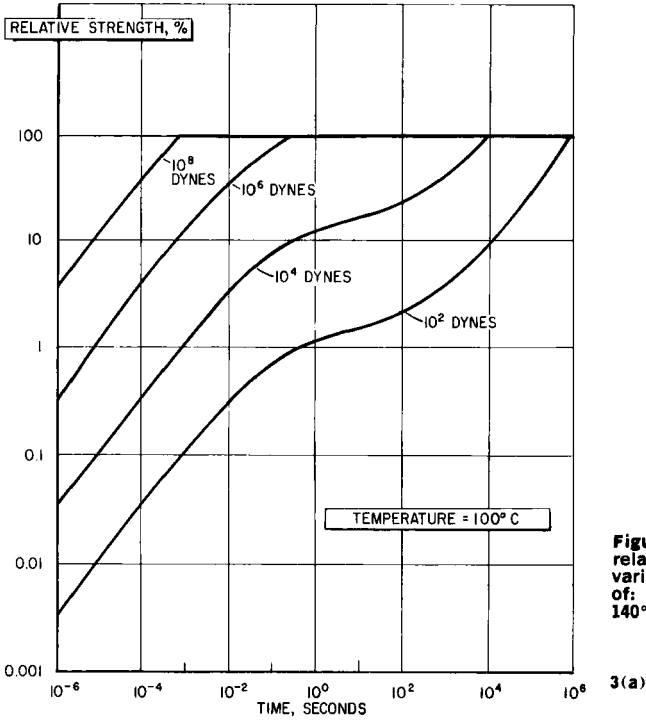
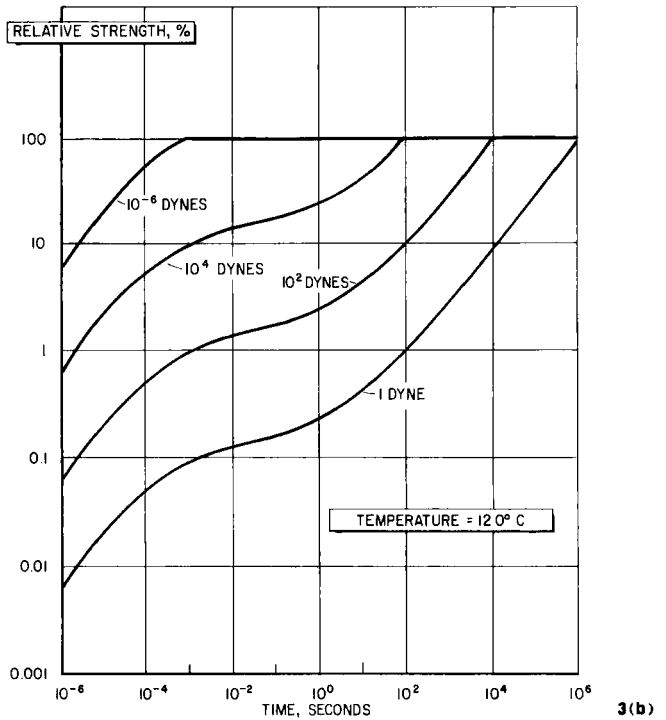
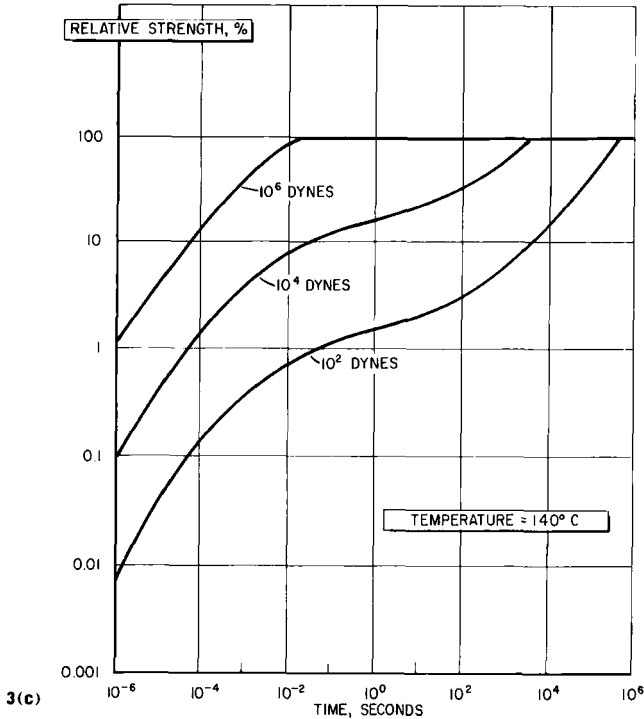


Figure 3. Plots of calculated relative strength vs. time for various loads and temperatures of: (a) 100°C, (b) 120°C, (c) 140°C.





### NOMENCLATURE

- $f, f', f''$  = force between units  
 $A$  = Hamaker constant  
 $d$  = separation  
 $r, r_0$  = distance  
 $F(r)$  = force which is grad of potential  
 $B$  = Lennard-Jones constant  
 $p$  = ratio of Lennard-Jones constants  
 $\theta$  = angle between normal and the line connecting two units  
 $x$  = normal distance between units  
 $l, m, n$  = integers  
 $\Sigma$  = summation  
 $s$  = exponent = 4 or 7  
 $a$  = cross-section area of a unit  
 $D$  = distance between units  
 $\sigma$  = stress or force/area  
 $p.s.i.$  = pounds per sq. in.

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