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A SIMPLE MODEL FOR EXPLOSIVES' FORMULATION

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ABSTRACT

A simple model based on surface chemistry is developed. This model is based on relatively simple concepts of contact angle, wetting and spreading. The results of the modeling can be stated by two simplified "rules of thumb": 1) A liquid will spread on the surface of a solid if the surface tension of the liquid is less than the surface free energy of the solid, and 2) The liquid having the surface tension nearest that of the solid will preferentially wet the surface of the solid. These two rules can then be used to define the parameters that constitute a process for formulating a plastic bonded explosive (PBX), which is a crystalline high-explosive material coated with a small amount of plastic polymeric material (the binder). The PBX then can be pressed to a high density, and machined to a specific shape. The pressed and machined explosive material can then be used in a physics experiment to study fundamental properties of either the explosive or some other material.

INTRODUCTION

Explosives can be formulated into a material appropriate for pressing into a high-density solid by coating the explosive crystals with a suitable plastic. The resulting composite or plastic-bonded explosive (PBX) can then be safely machined into a variety of shapes suitable for detonation physics experiments.

DEVELOPMENT

The formulation of a PBX represents a problem in surface chemistry that can be addressed using a simplified model based on the concept of contact angle. Figure 1 represents a drop of liquid resting on a uniform, perfectly flat solid surface.

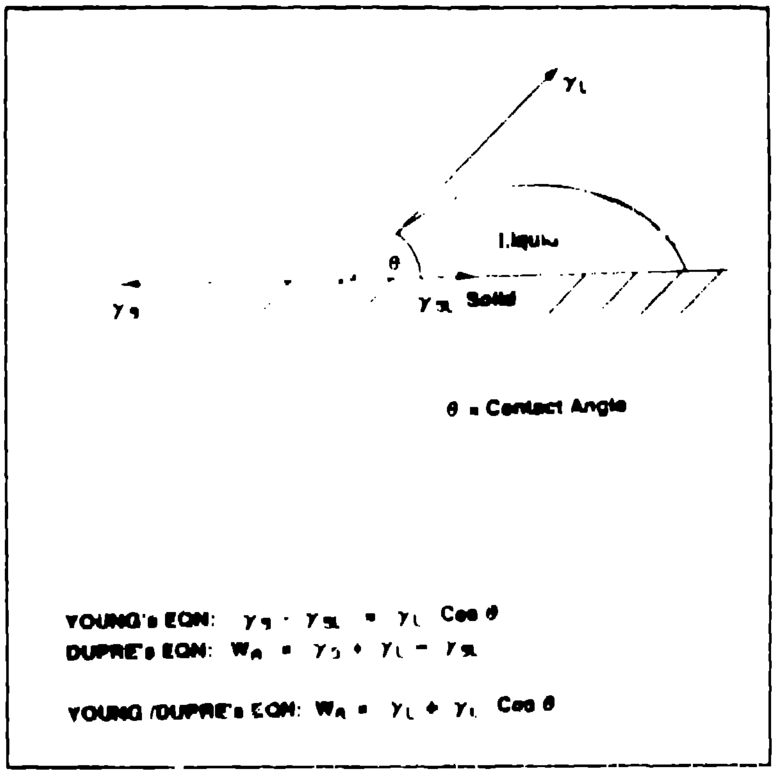

Figure 1 CONTACT ANGLE

In general the drop will not spread completely over the surface, but its edge will make an angle θ with the solid as shown in the figure. At its simplest, the theory of the contact angle allows us to resolve the equilibrium surface tensions that result in a stable droplet. The Young equation,

$$\gamma_s - \gamma_{sl} = \gamma_l \cos\theta, \qquad \text{Eqn. 1,}$$

where γ_s = solid surface tension, γ_L = liquid surface tension, and γ_{SL} = interfacial surface tension, is a statement of these results. The idea of contact angle is a rather practical concept since it can be measured using a variety of methods (see, for example, references 1, 2, and 3)..

The work of adhesion (W_A) measures the degree of wetting of a solid by a liquid. A high interfacial tension in a solid-liquid system indicates a low work of adhesion and conversely a low-interfacial tension is associated with a high work of adhesion.

The work of adhesion is defined by the equation

$$W_A = \gamma_S + \gamma_l - \gamma_{SL}, \qquad \text{Eqn. 2.}$$

Combining with Eqn. 1, we get the following equation:

$$W_A = \gamma_S + \gamma_l \cos \theta \qquad \text{Eqn. 3.}$$

The quantity $\gamma_S - (\gamma_{SL} + \gamma_L)$ is a measure of the driving force behind the spreading process and is usually called the spreading coefficient (S). The spreading coefficient is defined by the equation:

$$S = \gamma_S - (\gamma_{SL} + \gamma_l) \qquad \text{Eqn. 4.}$$

Thus, if S is positive, spreading can occur spontaneously; conversely, if S is negative the liquid will not spread spontaneously over the substrate.

We can see from Eqn. 4 that spreading is obtained as long as $\gamma_S > \gamma_L$. Under these conditions, the contact angle is zero, and Cos θ = 1. Thus, from Eqn. 3 we see that the work of adhesion increases as γ_l increases for a given solid surface.

The results of the modeling can be stated by two simplified "rules of thumb": 1) A liquid will spread on the surface of a solid if the surface tension of the liquid is less than the surface tension (free energy) of the solid, and 2) The liquid having the surface tension nearest that of the solid will preferentially wet the surface of the solid. These two rules can then be used to define the parameters that constitute a process for formulating a PBX.

DISCUSSION

An example of a process for producing PBXs is one known as the Water-Slurry Process. The Water-Slurry Process was developed at Los Alamos about 1948 for producing HMX-based PBXs. HMX is a high explosive commonly used in the explosives industry. Figure 2 is a diagram representing the Water-Slurr Process in terms of surface tension.

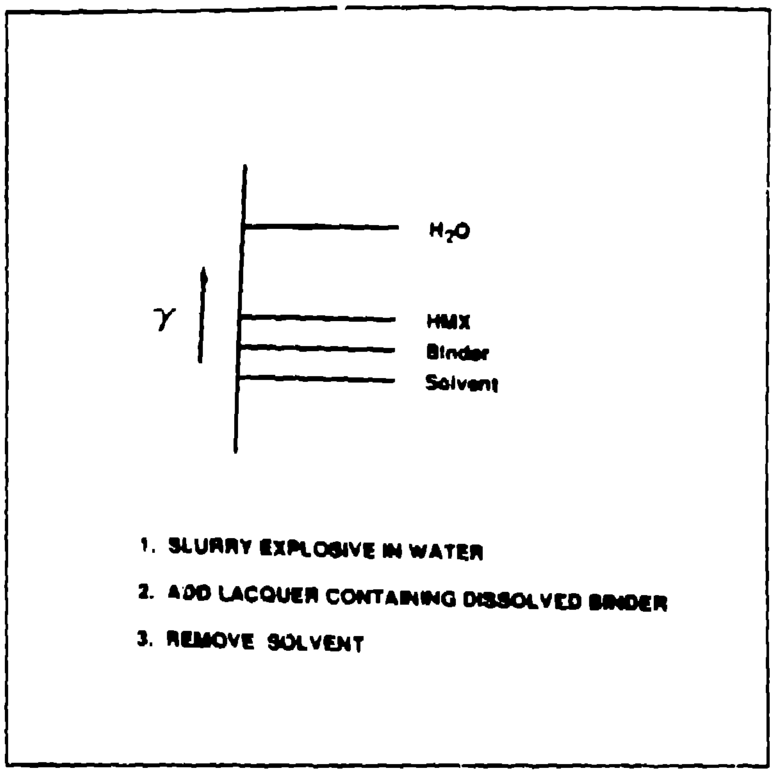

Figure 2 WATER-SLURRY PROCESS

In the Water-Slurry Process, the explosive is first mixed into a stirred pot containing a large volume of water. Since the HMX has a surface tension less than that of the water, the water has no affinity for the surface of the HMX. The slurry is stirred until a good dispersion of the HMX is made in the water. A lacquer, containing the binder dissolved in a volatile solvent is poured into the slurry and mixing is continued. The solvent is removed by distillation leaving behind the polymeric binder. The binder having a surface tension less than that of the HMX has an affinity for its surface, and subsequently coats on the surface of the high explosive. The closer the binder surface tension is to that of the HMX, the better the coating. The coated HMX is filtered and dried, and a PBX is produced.

The PBX then can be pressed to a high density, and machined to a specific shape. The pressed and machined explosive material can then be used in a physics experiment to study some fundamental properties of the explosive or to study the properties of shocked material.

CONCLUSION

We have seen that the process for producing a PBX can be analyzed in terms of simple surface chemistry concepts. Changes in the process to accommodate different types of binders, explosives, etc., can be made based on predictions made using the model. The model can also be useful in the design of other coating processes.

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