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*Title:* A Probabilistic, Semi-Empirical Approach to Modeling  
Diffusion Bond Strength

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## A Probabilistic, Semi-Empirical Approach to Modeling Diffusion Bond Strength

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### Introduction

Manufacture of critical diffusion bonded components could benefit from predictive models of diffusion bond joint strength. Existing models (e.g. Ref.s 1,2,3) focus on porosity closure, which is a necessary but not sufficient condition for acceptable joint strength. The present work identifies unmodeled dynamics intrinsic to manufacturing but not captured in existing models. Controls regulating these dynamics are proposed, and the topography of real engineering surfaces is described by distribution functions. Pore closure kinetics *then* can successfully link initial surface topography and final porosity distribution, which in turn correlates to joint strength given experimental data linking porosity to joint strength.

### Procedure

Unmodeled dynamics in current diffusion bond models include:

- mechanical constraints affecting plastic flow
- micro-scale constitutive behavior (asperities same scale as grains)
- material texture and grain orientation
- topography of real engineering surfaces : waviness, parallelism, and micro-roughness
- contamination

A complete phenomenological description of all these effects does not presently exist, but in-process engineering controls are suggested that ensure run-to-run consistency. Monte Carlo pore closure models are used to first correlate topography to the final porosity distribution. Given additional data relating joint impact strength and porosity, the link between process inputs and bond strength is finally made.

## Results and Discussion

This work directly addresses the issue of paramount importance in the manufacture of a critical diffusion-bonded component: *joint strength*. The approach is semi-empirical however, since it relies on a well-characterized set of experiments linking porosity to joint strength (Ref. 4 was used for this work), all other intervening factors held constant. These intervening factors or unmodeled dynamics cause discrepancies between existing pore closure models and real manufacturing situations; the pore closure models are well validated under controlled laboratory conditions, but generally fair poorly when compared to production data. The second major contribution of this work is the identification of in-process controls that allow for greater control over unmodeled dynamics in actual production situations, in which case pore closure models *then* have greater relevance and predictive power.

The third principal contribution of this work is a generalization of existing pore closure models to account for the topography of real engineering surfaces by considering distributions of initial pore sizes that result when two engineering surfaces come into contact. The sintering time for any given initial pore size may be calculated from simple pore closure models, and Monte Carlo methods are then used to generate the *distribution* of final porosity remaining in the bond. If a well-characterized data set exists relating porosity to joint impact strength, which is the strength parameter most sensitive to porosity, then the distribution of bondline porosity can be translated into a distribution of joint strengths for a given bonded article. Using this strength distribution, a probabilistic life prediction approach is possible, along with an assessment of the sensitivity of part life to changes or fluctuations in the manufacturing process. Also, the inverse problem is addressed: given a desired joint strength, what manufacturing processing parameters are required.

## Conclusion

A new probabilistic, semi-empirical model for diffusion bond joint strength is proposed, and its application to realistic manufacturing situations is considered in detail. It is shown that the new model is better able to account for the effect of manufacturing process variables on diffusion bond joint strength. In addition to providing guidance in manufacturing process development, it is expected that the present model will be of practical utility in determining 'retirement-for-cause' criteria for critical diffusion-bonded articles.

## Acknowledgements

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## References

1. Guo, ZX, Ridley, N, 1987. Modeling of diffusion bonding of metals. *Materials Science and Technology*, Vol. 3(11): p. 945 to 953.
2. Takahashi, Y, Inoue, K, 1992. Recent void shrinkage models and their applicability to diffusion bonding. *Materials Science and Technology*, Vol. 8(11): 953 to 964.
3. Hill, A, Wallach, ER, 1989. Modeling solid-state diffusion bonding. *Acta Metallurgica*, Vol. 37(9): 2425 to 2437.
4. Ohsumi, M et al, 1985. The application of diffusion welding to aircraft titanium alloys. *Trans. Iron and Steel Inst. of Japan*, Vol. 25(6): 513 to 520.

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# A Probabilistic, Semi-Empirical Approach to Modeling Diffusion Bond Strength

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# Motivation

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- Solid-state diffusion bonding is a deceptively simple process
  - Diffusion bonding is joining at it simplest and process control at its potentially most challenging!
  - root cause analysis can be extremely difficult if based purely upon destructive evaluation
- Process modeling can be useful for both process control and optimization
- Existing models do not capture certain aspects of real parts or manufacturing processes that have an impact on final joint quality



# Concise Review of Previous Models

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- First phenomenological model due to King and Owczarski (P&W, 1967-68)
  - generated insights that have guided much later work
  
- Garmong, Paton & Argon (1975)
  - first model to consider multiple deformation / void closure mechanisms and surface topography
  
- Derby, Hill and Wallach (1982 - 89) and
- Pilling, Ridley, et al (1984-87)
  - several articles that have extended early work of Garmong et al by introducing a plethora of pore closure mechanisms and multiple deformation modes - strong analogies to pore closure models for sintering



# Shortcomings of Current Models

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- Current models describe the evolution of bond area and the associated elimination of bondline porosity, which is NOT the same as modeling bond strength
- Current models suffer from an unrealistic rendering of the topography of real surfaces



# Shortcomings of Current Models

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- Current models do not take into account bondline contamination and residual gases at the bondline
- Current models do not consider material texture, thermomechanical processing, and the possible interactions of grain growth kinetics and plastic deformation
- Current models do not take into account surface deformation caused by residual stresses or stress triaxiality at the interface



# Approach in this Work

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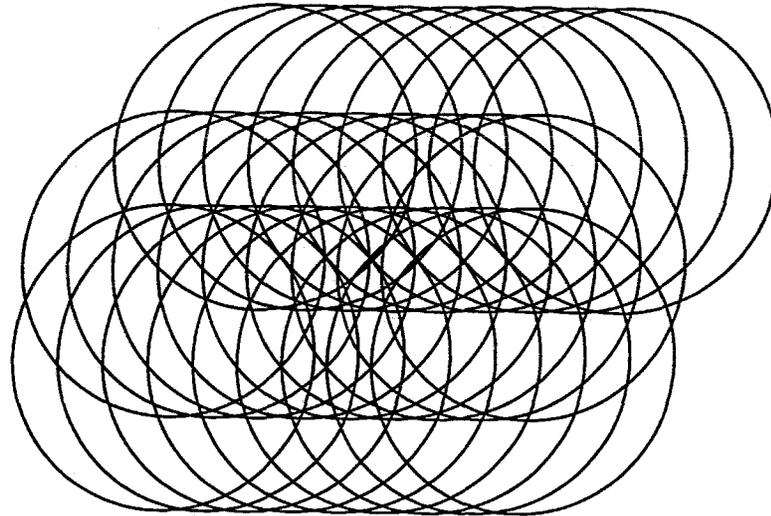
- This work will address *two* of the shortcomings of current models:
  - model for joint strength
    - semi-empirical model combining experimental studies and modeling work
    - final model attempts to link processing conditions to bond impact strength
  - realistic representation of contacting surfaces
    - statistical treatment of surfaces
  - A theoretical framework for incorporating these effects will be postulated
  - *This framework has more general applicability as an example of how to use physics-based models in conjunction with statistical methods to model manufacturing processes*



# Topography of Real Engineering Surfaces

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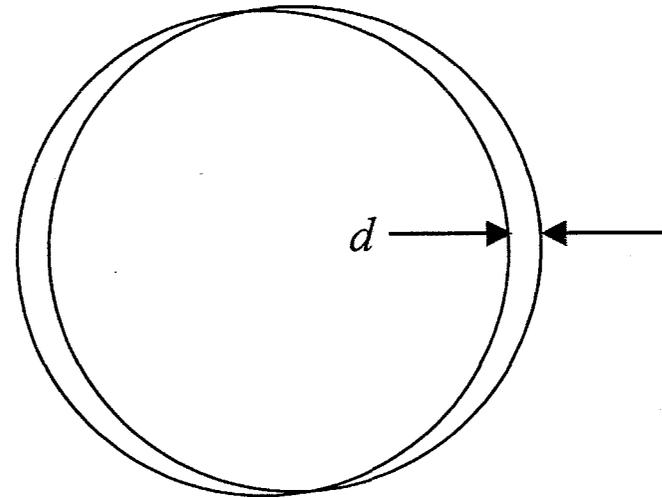
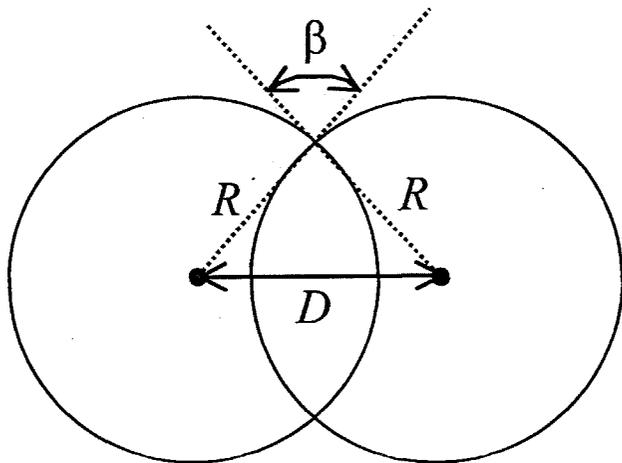
- Materials are prepared by machining using rotary machining tools (millers, cutters, etc.)



*Schematic of overlapping machining marks*

# Topography of Real Engineering Surfaces

- contact between real engineering surfaces is a problem of intersecting contact between multiple circular machining marks
- THREE important parameters - contact angle  $\beta$ , spacing of marks  $D$ , and advance rate  $d$



$$(d, \text{inches}) = \frac{(\text{feed rate, ipm})}{(\text{spindle speed, rpm})} \cdot (1 \text{ rev})$$

# Topography of Real Engineering Surfaces

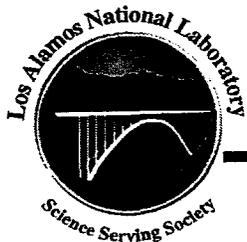
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- From elementary geometry, we find that

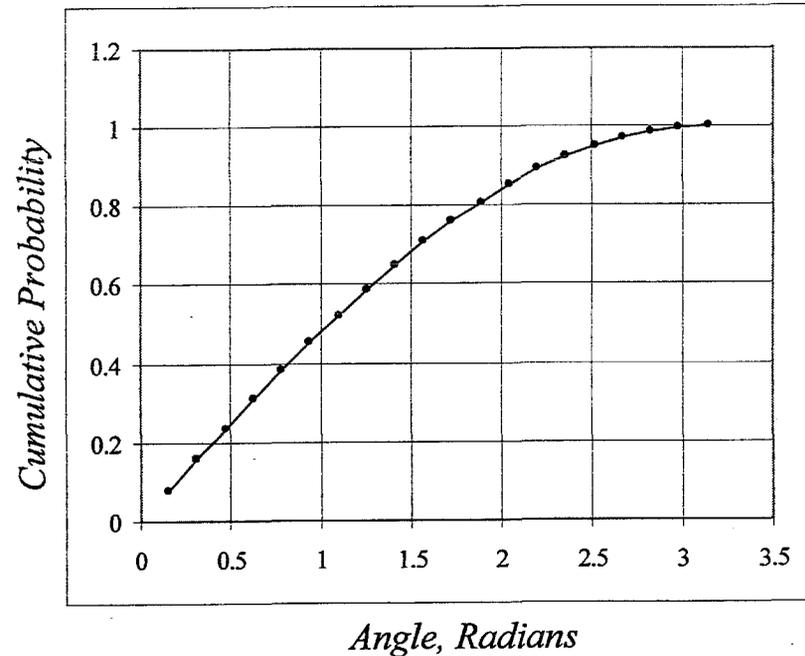
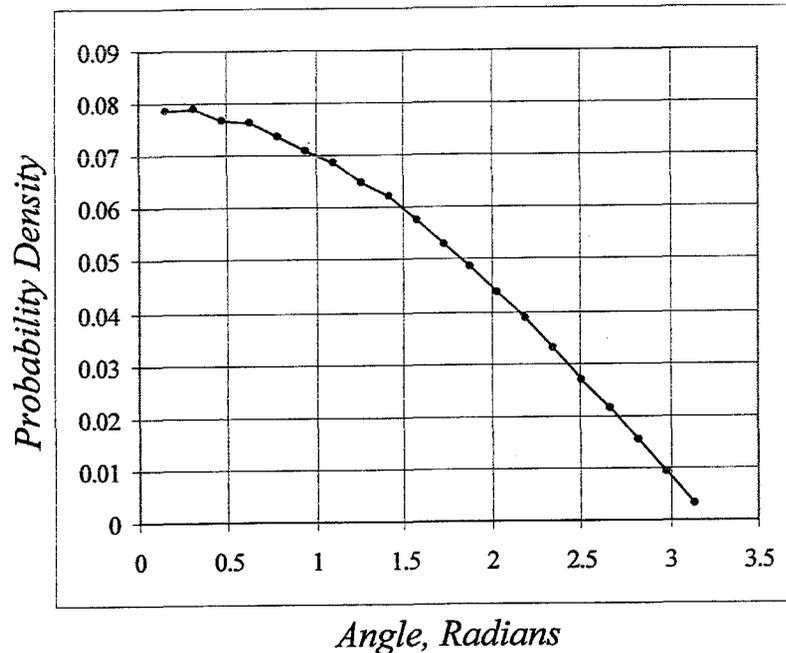
$$\beta = \pi - 2 \cdot \tan^{-1} \left[ \sqrt{\frac{1}{\phi^2} - 1} \right]$$

$$\text{where } \phi \equiv \frac{D}{2R}, 0 \leq \phi \leq 1$$

- Since the spacing is arbitrary, to find the distribution of  $\beta$  we assume that  $\phi$  is a uniformly distributed random variable and perform Monte Carlo Analysis to find the probability density function (PDF) for  $\beta$

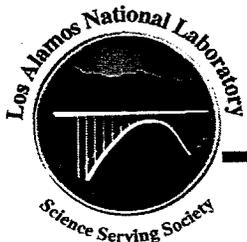


# PDF and CDF for Contact Angle



*NOTE: Probability Density has been normalized*

*Details of Monte Carlo Calculations: 30,000 trials per run, 9 runs used to get average PDF, which was assembled by using histogram with bin width of 0.157 radian, CDF calculated from average PDF*



# Incorporating Effect of Machining Parameters

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- The advance rate  $d$  is assumed to have a normal distribution about its mean:

$$f_d(d) = \frac{1}{\sigma_d \sqrt{2\pi}} \exp\left[-\frac{(d - \bar{d})^2}{2\sigma_d^2}\right]$$

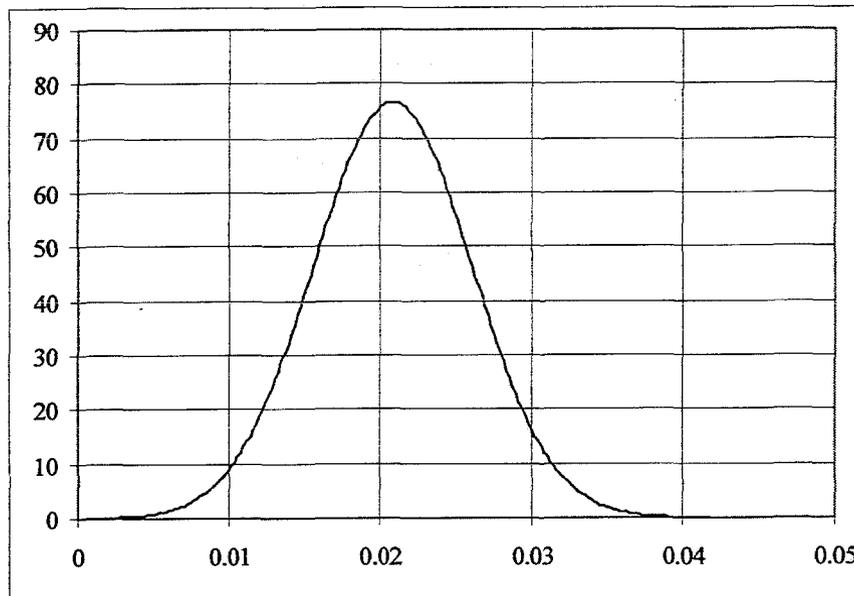
- The corresponding CDF is:

$$F_d(d) \equiv \int_{-\infty}^d f_d(t) dt = \frac{1}{2} \left\{ 1 + \operatorname{erf} \left[ \frac{(d - \bar{d})}{\sqrt{2} \cdot \sigma_d} \right] \right\}$$



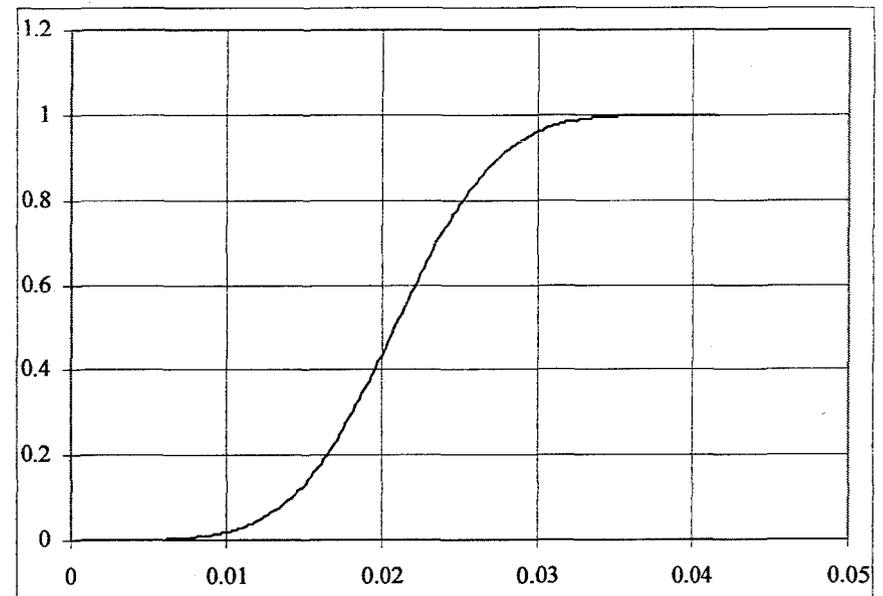
# Incorporating Effect of Machining Parameters

*Probability Density Function*



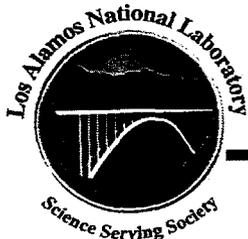
*d, inches*

*Cumulative Distribution Function*



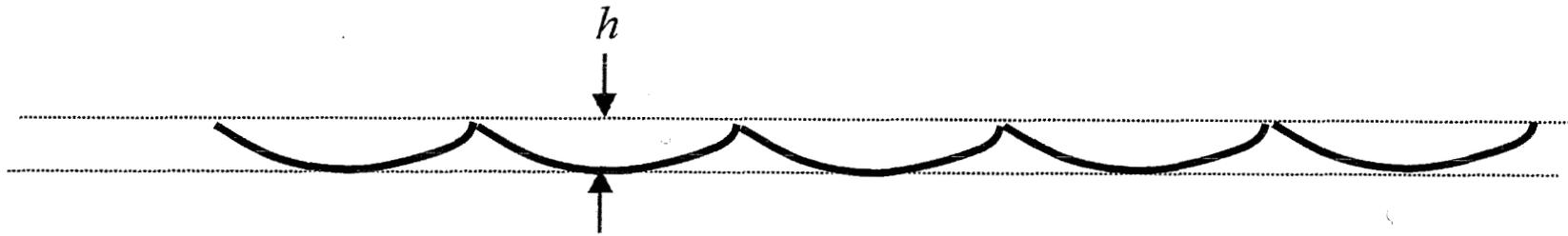
*d, inches*

Details of Machining Parameters: feed rate = 25 ipm,  
spindle speed = 1200 rpm,  $d_{mean} = 0.021$  in,  $\sigma = 0.005$  in



# Incorporating Effect of Machining Parameters

- The surface roughness feature peak-to-valley height,  $h$ , will also be assumed to obey a normal distribution:

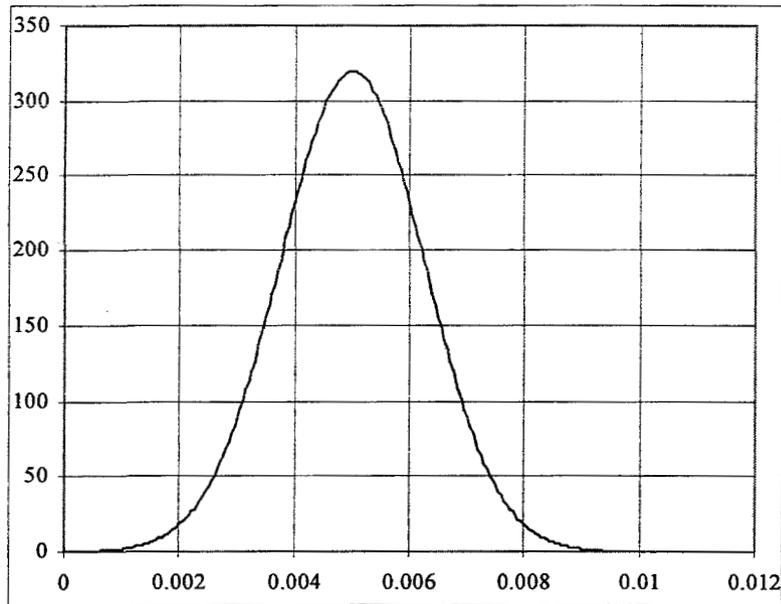


$$f_h(h) = \frac{1}{\sigma_h \sqrt{2\pi}} \exp\left[-\frac{(h - \bar{h})^2}{2\sigma_h^2}\right]$$

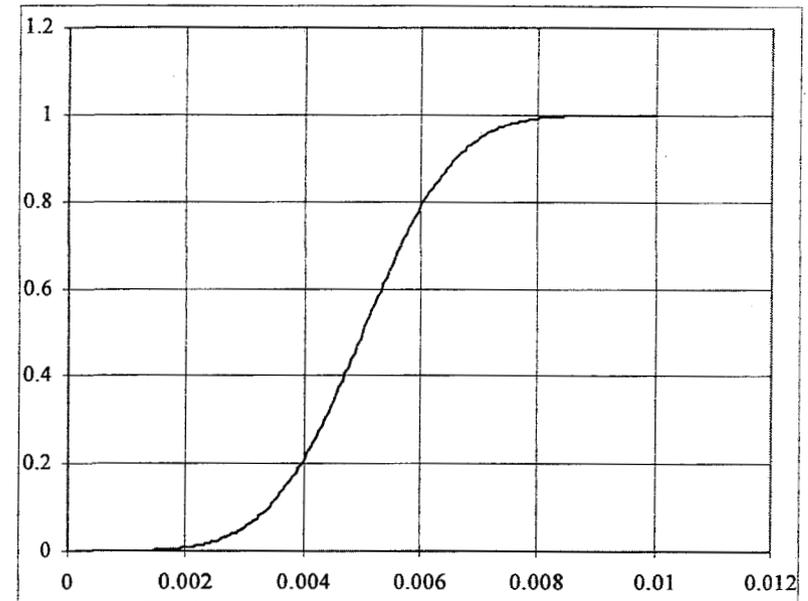
$$F_h(h) \equiv \int_{-\infty}^h f_h(t) dt = \frac{1}{2} \left\{ 1 + \operatorname{erf} \left[ \frac{(h - \bar{h})}{\sqrt{2} \cdot \sigma_h} \right] \right\}$$

# Incorporating Effect of Machining Parameters

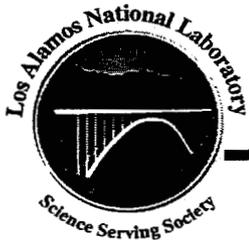
*Probability Density Function*



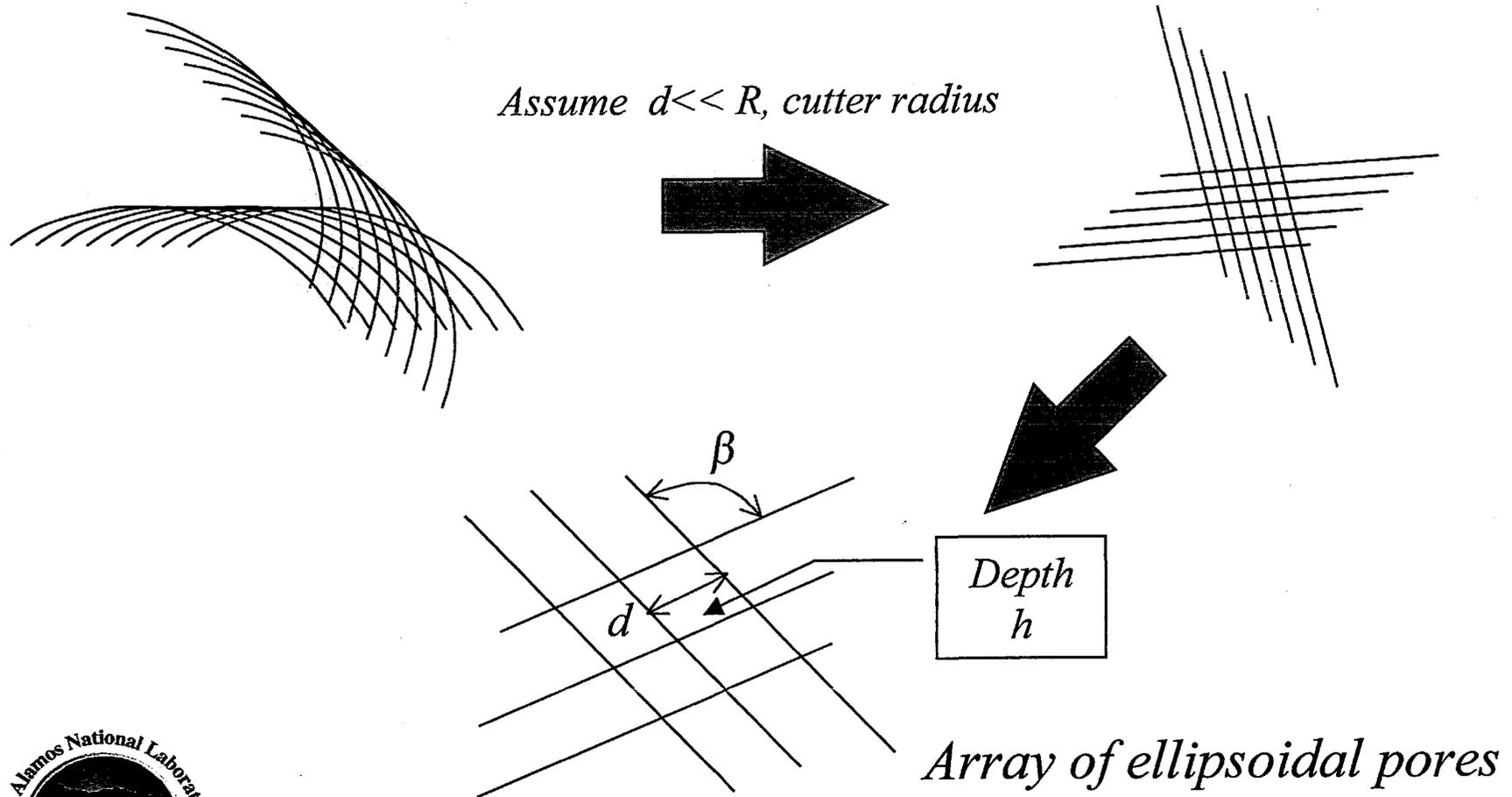
*Cumulative Distribution Function*



$$h_{mean} = 0.005 \text{ in}, \quad \sigma = 0.00125 \text{ in}$$



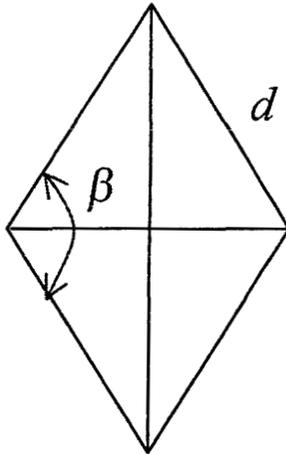
# Utilizing $\beta$ , $d$ and $h$ to Model Initial Pore Distribution



# Utilizing $\beta$ , $d$ and $h$ to Model Initial Pore Distribution

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- Calculate an equivalent pore radius for a spherical pore having the same volume as the ellipsoidal pores:



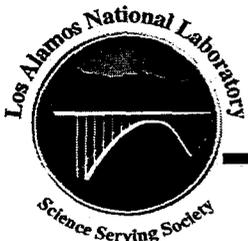
$$\frac{4}{3}\pi r_{eq}^3 = \frac{4}{3}\pi h d^2 \cos\left(\frac{\beta}{2}\right) \cdot \sin\left(\frac{\beta}{2}\right)$$

$$\text{so } r_{eq} = \sqrt[3]{h d^2 \cos\left(\frac{\beta}{2}\right) \cdot \sin\left(\frac{\beta}{2}\right)}$$

# Common “Trick” used in this Work

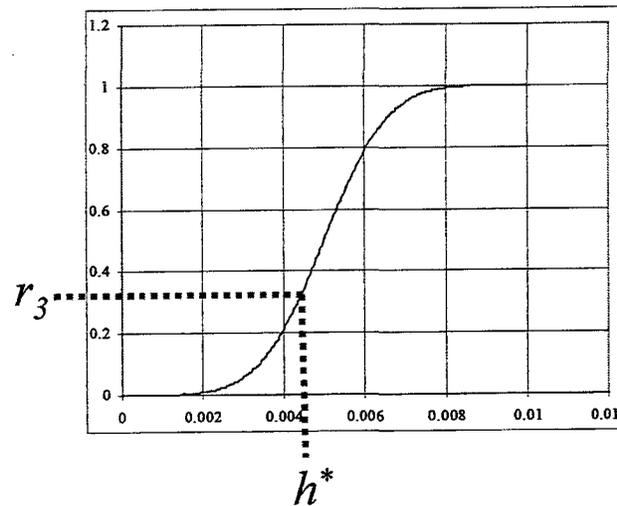
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- Use Monte Carlo approach to generate a PDF for a given quantity  $\beta$  (in this case the contact angle)
- Sum PDF to get a CDF, or cumulative distribution function for  $\beta$
- For subsequent Monte Carlo Calculations involving the quantity  $\beta$ , use a “roulette wheel” selection method where a random number is used to represent a probability of selection, and the CDF for  $\beta$  provides the value of  $\beta$  corresponding to the randomly chosen selection probability.



# Utilizing $\beta$ , $d$ and $h$ to Model Initial Pore Distribution

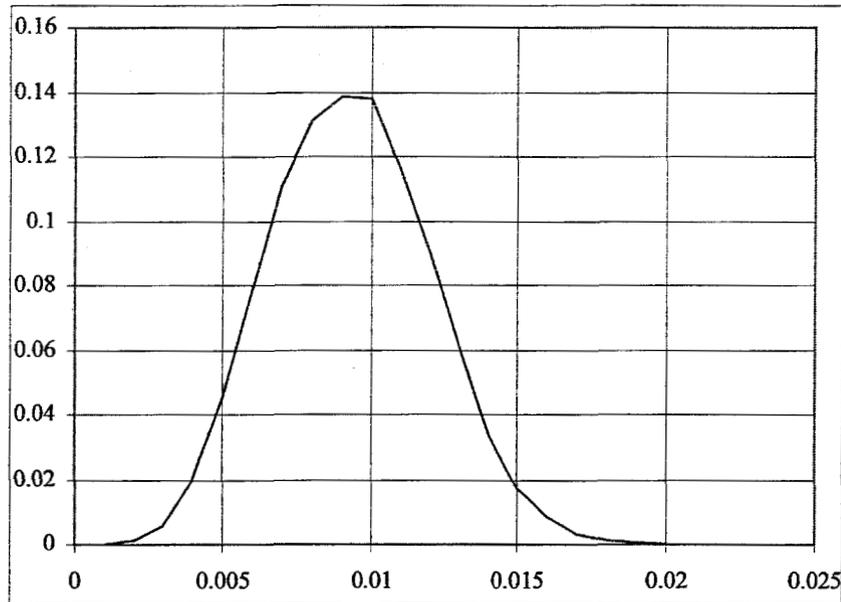
- Generate initial pore distribution as follows:
  - generate a random number array  $(r_1, r_2, r_3)$  on the interval  $r_i \in [0, 1]$
  - given the CDFs for  $\beta$ ,  $d$ , and  $h$ , use the random numbers to select  $\beta^*$ ,  $d^*$ , and  $h^*$ :



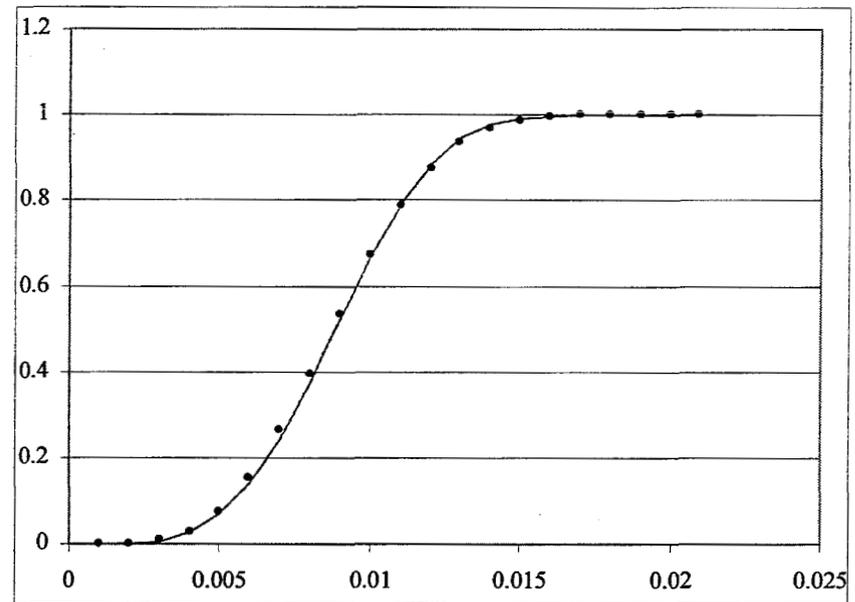
- use the relationship between  $r_{eq}$  and  $\beta$ ,  $d$ , and  $h$
- Iterate in Monte Carlo fashion to get distribution for  $r_{eq}$

# Utilizing $\beta$ , $d$ and $h$ to Model Initial Pore Distribution

*Normalized PDF*



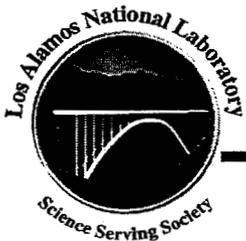
*CDF*



*CDF well-represented by a Weibull Distribution:*

*Shape parm. = 3.4, Scale parm. = 0.00875, Loc. parm. = .001*

*Details of Monte Carlo Calc.: CDFs for  $d$ ,  $h$ , and  $\beta$  used to generate PDF for initial pore size, 10,000 trials per run, 9 runs.*



# Incorporating Physics of Pore Closure and Bonding Process Parameters

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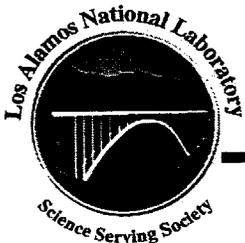
*Example of multiple mechanism physics-based model for pore closure resulting in non-linear ordinary differential equations (ODEs)*

*Model due to Garmong, Paton and Argon, 1975*

$$\left(\frac{dr}{dt}\right)_{total} = -\left\{\left(\frac{dr}{dt}\right)_{creep} + \left(\frac{dr}{dt}\right)_{vacancy\ diffusion}\right\}$$

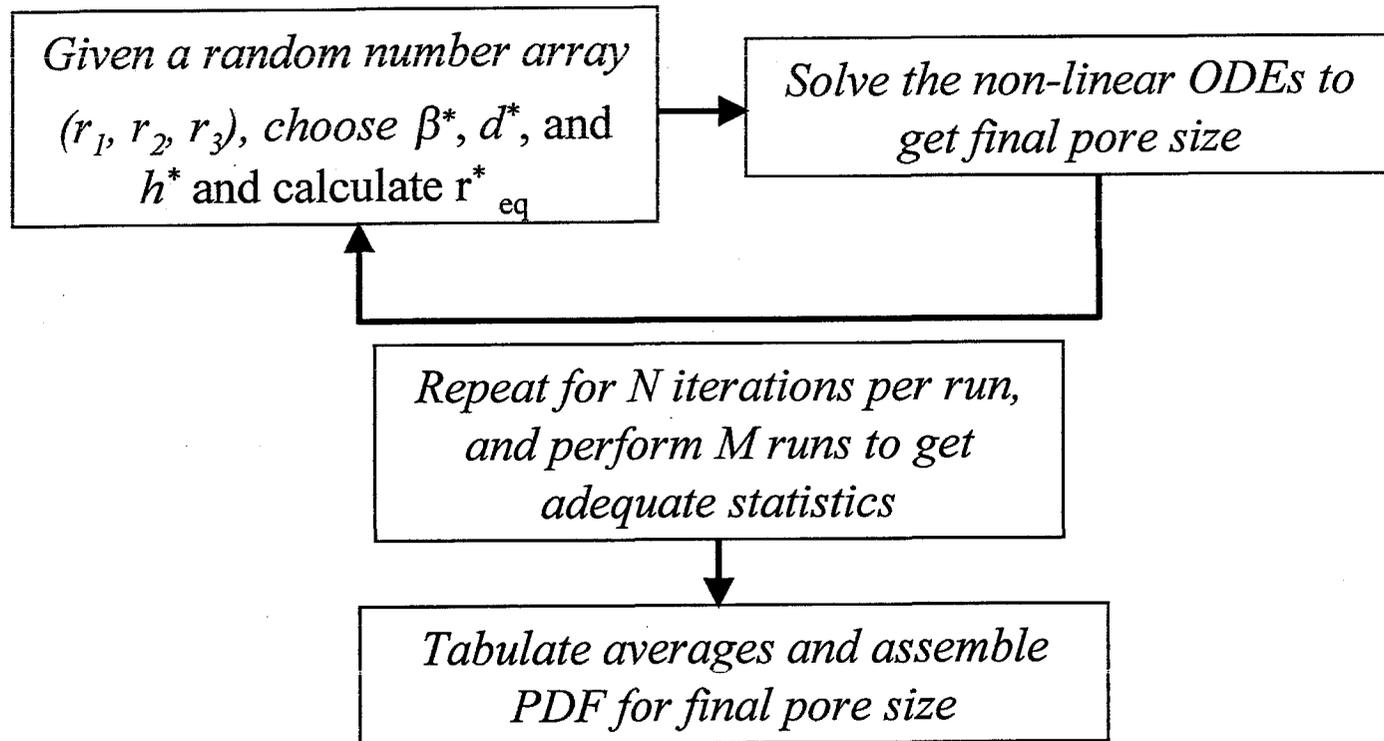
$$\left(\frac{dr}{dt}\right)_{creep} = \frac{3K_1}{4} r \left[ 2\sigma_0 \ln\left(\frac{b_0}{r}\right) + \left(\frac{2\gamma}{r} - P_i + P_{ext}\right) \right]$$

$$\left(\frac{dr}{dt}\right)_{vacancy\ diffusion} = \left(\frac{D_v \Omega}{kT}\right) \cdot \frac{1}{r} \cdot \left(\frac{2\gamma}{r} + P_{ext}\right)$$



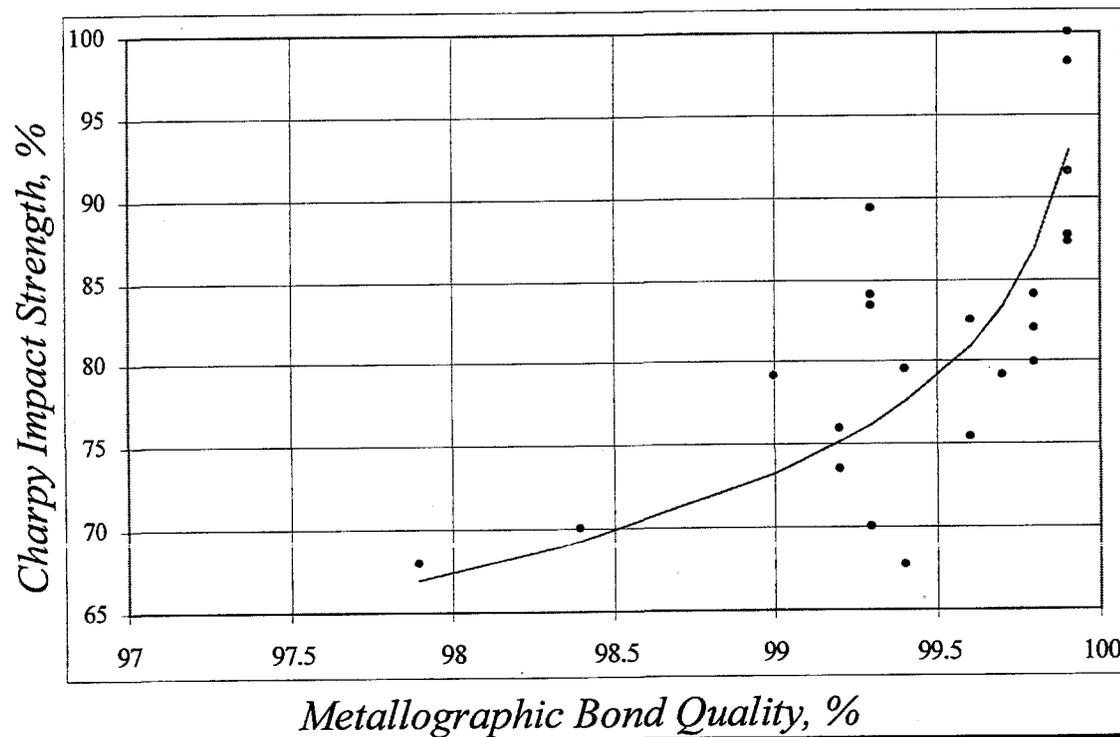
# Incorporating Physics of Pore Closure and Bonding Process Parameters

- Monte Carlo method of finding final pore size distribution:



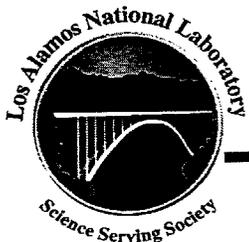
# Modeling Bond Strength

- **Needed:** careful set of experiments linking final pore size to impact strength
  - Difficult to do since above 80% impact, the bond is practically parent metal!



*Data shown for  
diffusion-bonded*

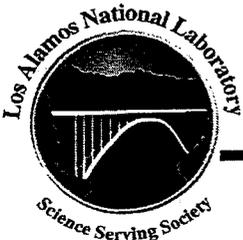
*Ti-6Al-4V*



# Modeling Bond Strength

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- Assume the existence of a careful set of experiments, i.e. a ‘master curve’ correlating metallographic bond quality to impact strength, THEN
  - the final pore size distribution can be ‘mapped’ into a distribution of impact strengths to be expected
- This then completes the series of calculations, and now bond impact strength has been related to:
  - realistic surface topography
  - machining conditions
  - bond conditions
  - ASSUMING of course that other effects are ‘held constant,’ like cleanliness!



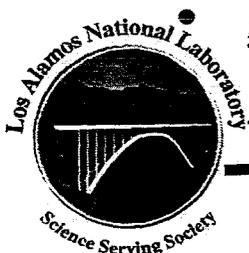
# Conclusions and Future Work

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- This theoretical framework has allowed the following effects to be included
  - realistic rendering of topography and contact of real engineering surfaces
  - effects of machining
  - effects of bond parameters
  - generalization of physics-based pore closure models to operate on a distribution of initial pore sizes, i.e. a distribution of initial conditions for the ODEs
  - a means to link to bond strength given additional empirical data on the relationship between final pore size and bond strength

*SO, ultimately this model allows bond strength to be linked to manufacturing process variables*

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# Conclusions and Future Work

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- Work in Progress:
  - Monte Carlo computation to link initial pore size distribution to final pore size distribution through use of physics-based pore closure models
  - final correlation to experimental data for Ti-6Al-4V - compare predicted joint strength distribution to actual joint strength distribution
  - automation of procedures to facilitate future use of model and extension to other materials

