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# PREDICTIVE MATERIAL

# modeling:

combining fundamental  
physics understanding,  
computational methods,  
and empirically  
observed behavior

*Technical Editor(s):*

Mark T. Kirk and M. Erickson Natishan



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***Predictive Material Modeling:  
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Understanding, Computational  
Methods and Empirically  
Observed Behavior***

*M. T. Kirk and M. Erickson Natishan, editors*

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## Foreword

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The Symposium on Predictive Material Modeling: Combining Fundamental Physics Understanding, Computational Methods and Empirically Observed Behavior was held in Dallas, Texas on 7–8 November 2001. ASTM International Committee E8 on Fatigue and Fracture sponsored the symposium. Symposium chairpersons and co-editors of this publication were Mark T. Kirk, U. S. Nuclear Regulatory Commission, Rockville, Maryland and MarjorieAnn Erickson Natishan, Phoenix Engineering Associates, Incorporated, Sykesville, Maryland.

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# Overview

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An ASTM International Symposium concerning *Predictive Material Modeling: Combining Fundamental Physics Understanding, Computational Methods, and Empirically Observed Behavior* was held on 7–8 November 2001 in Dallas, Texas in conjunction with the semi-annual meetings of ASTM International Committee E8 on Fracture and Fatigue. The symposium was motivated by the focus of many industries on extending the design life of structures. Safe life extension depends on the availability of robust methodologies that accurately predict both the fundamental material behavior and the structural response under a wide range of load conditions. Heretofore, predictive models of material behavior have been based on empirical derivations, or on fundamental physics-based models that describe material behavior at the nano- or micro-scale. Both approaches to modeling suffer from issues that limit their practical application. Empirically-derived models, while based on readily determined properties, cannot be reliably used beyond the limits of the database from which they were derived. Fundamental, physically-derived models provide a sound basis for extrapolation to other materials and conditions, but rely on parameters that are measured on the microscale and thus may be difficult and costly to obtain. It was the hope that this conference would provide an opportunity for communication between researchers pursuing these different modeling approaches.

The papers presented at this Symposium included six concerning ferritic steel; these address fracture in the transition regime, on the upper shelf, and in the creep range. Three of these papers used a combination of the Gurson and Weibull models to predict fracture performance and account for constraint loss. While successful at predicting conditions similar to those represented by the calibration datasets, all investigators found the parameters of the (predominantly) empirical Weibull model to depend significantly on factors such as temperature, strain rate, initial yield strength, strain hardening exponent, and so on. These strong dependencies make models of this type difficult to apply beyond their calibrated range. Natisan proposed the use of physically derived models for the transition fracture toughness of ferritic steels. While this approach shows better similarity of parameters across a wide range material, loading, and temperature conditions than does the Weibull approach, it has not yet been used to assess constraint loss effects as the Weibull models have.

Three papers at the Symposium addressed topics un-related to steels. One paper applied the Weibull models used extensively for steel fracture to assess the interfacial fracture of electronic components. As is the case for steel fracture, the Weibull models predict well conditions similar to the calibration dataset. In the remaining two papers researchers affiliated with the Naval Research Laboratory used advanced computational and experimental techniques to develop constitutive models for composite and shape memory materials.

We would like to close this overview by extending our thanks not only to the authors of the papers you find in this volume, but also to the many peer reviewers, and to the members of the ASTM International staff who made publication of this volume possible.

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