Computational Methods in Materials Characterisation
High Performance Structures and Materials

Objectives

The High Performance Structures and Materials series has been established to document the dynamic and rapid changes presently happening in the field of structural engineering. New concepts are constantly being introduced, and the series reflects the wide range of significant international research and development.

The series encompasses the following topics:

- High Performance Structures
- Nonlinear Structural Behaviour
- Emerging Applications
- Design Innovation
- Smart Structures
- Space Structures
- Microstructures
- Marine and Offshore Structures
- Composite Structures
- Retrofitting of Structures
- Sustainability in Design
- Shape and Topology Optimisation
- Shock and Impact
- Structural Capacity under Damage
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Computational Methods in Materials Characterisation

Editors

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University of New Mexico, USA

C.A. Brebbia
Wessex Institute of Technology, UK
Materials have played major roles in directing the course of history. Today, materials can play an equally significant part, by improving quality of life, while at the same time becoming more accessible, at a lower environmental and economic cost. Materials characterization is an important aspect of this process. According to the definition of the ASM International Materials Characterization Handbook, ‘Characterization describes those features of composition and structure (including defects) of a material that are significant for a particular preparation, study of properties, or use, and suffice for reproduction of the material.’ New materials are being developed that are lighter, stronger, and require less energy to produce than existing materials. Others are used in more durable and more bio-compatible implants. Yet others are traditional materials whose structure and behavior is made more complex by recycling.

To achieve better performance (mechanical, energetic, thermal, etc.), the structure of many materials is becoming increasingly complex, to the point where simple mathematical models and experimental methods are inadequate for the understanding and characterization of their properties. Structure is probably the single most important factor deciding the behavior of a material, be it mechanical, thermal, optical, electrical or chemical. Often the structure depends on the processing history, and thus the material must be characterized in two states of its life, fluid and solid. Computers have become almost essential in assisting the scientist or engineer in the characterization of materials that are in use, under development, or more interestingly purely abstract concepts.

In many cases, computer models are complementary to experimental measurements. For example, one can characterize the morphology and chemical behavior of bone material, and then attempt to reproduce the same characteristics in an artificial material that can be prepared and implanted readily. Computers can then help in determining whether the mechanical behavior of the artificial material is adequate for the application and perhaps in modifying it to optimize certain properties, or one may be interested in characterizing the damage sustained by a particular sample, and then model the material to investigate the failure mechanisms that lead to this damage, again with the betterment of the material in view.

This book comprises most of the papers presented at the 1st International Conference on Material Characteristics held in Santa Fe, New Mexico. It brings together the work of practitioners in many fields of engineering,
materials and computational science, and especially links experimentalists and modelers. It was felt that in many cases, experimentalists may not be aware of certain computational methods, while at the same time modelers may find a new application which is well suited to their simulation work. By such an interaction, new collaborations, opportunities and ideas may be established, which will ultimately result in scientific advances.

The editors wish to acknowledge the invaluable help of the international scientific advisory committee, for their work in obtaining, selecting and in many cases providing excellent contributions to the conference.

The Editors,
Santa Fe
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